

10/767784

=> file registry

FILE 'REGISTRY' ENTERED AT 13:51:39 ON 02 MAY 2007

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STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

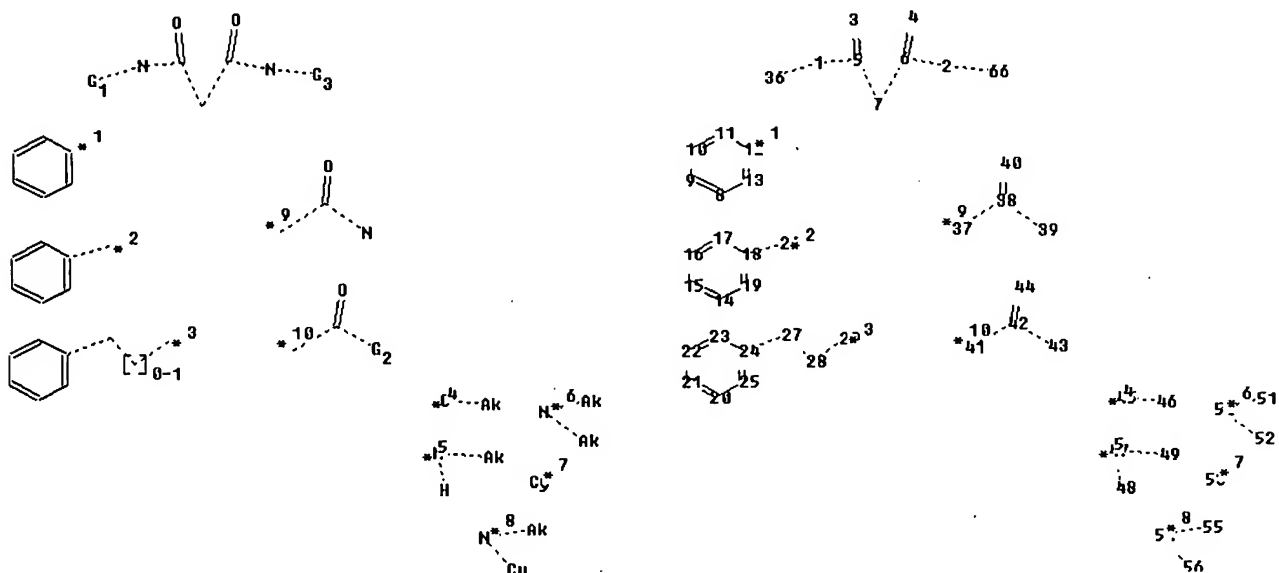
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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<http://www.cas.org/support/stngen/stndoc/properties.html>

Uploading L1.str



chain nodes :

1 2 3 4 5 6 7 36 40 41 42 43 44 45 46 47 48 49 50 51 52 53
54 55 56 66

ring nodes :

8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 37 38 39

ring/chain nodes :

```

26 27 28 29
chain bonds :
1-5 1-36 2-6 2-66 3-5 4-6 5-7 6-7 18-26 24-27 38-40 41-42 42-43 42-44
45-46 47-48 47-49 50-51 50-52 54-55 54-56
ring/chain bonds :
27-28 28-29
ring bonds :
8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17 17-18 18-19 20-
21
20-25 21-22 22-23 23-24 24-25 37-38 38-39
exact/norm bonds :
1-5 1-36 2-6 2-66 3-5 4-6 5-7 6-7 18-26 24-27 27-28 28-29 37-38 38-39
38-40 41-42 42-43 42-44 45-46 47-48 47-49 50-51 50-52 54-55 54-56
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17 17-18 18-19 20-
21
20-25 21-22 22-23 23-24 24-25

```

G1:[*1],[*2],[*3]

G2:[*4],[*5],[*6],[*7],[*8]

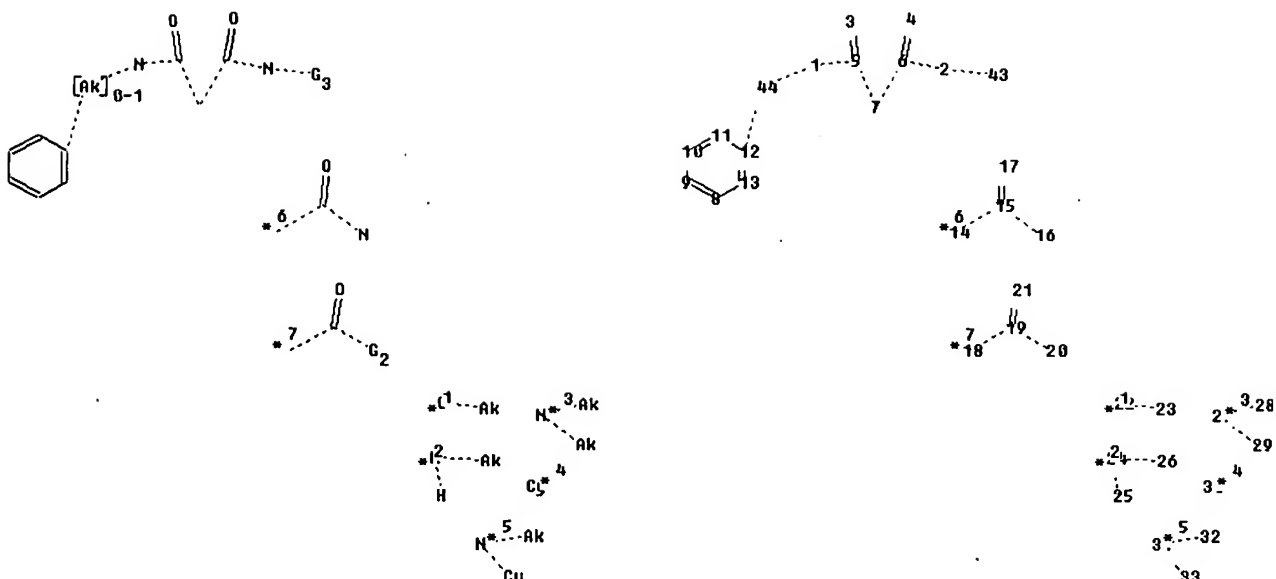
G3:[*9],[*10]

```

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS 29:CLASS
36:CLASS 37:Atom
38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS
46:CLASS 47:CLASS
48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:Atom 54:CLASS 55:CLASS
56:Atom 66:CLASS

```

Uploading L9.str



```

chain nodes :
1  2  3  4  5  6  7  17  18  19  20  21  22  23  24  25  26  27  28  29  30  31
32 33 43 44
ring nodes :
8  9  10 11 12 13 14 15 16
chain bonds :
1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 15-17 18-19 19-20 19-21 22-23
24-25 24-26 27-28 27-29 31-32 31-33
ring bonds :
8-9 8-13 9-10 10-11 11-12 12-13 14-15 15-16
exact/norm bonds :
1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 14-15 15-16 15-17 18-19 19-20
19-21 22-23 24-25 24-26 27-28 27-29 31-32 31-33
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13
isolated ring systems :
containing 8 :

```

```
G2: [*1], [*2], [*3], [*4], [*5]
```

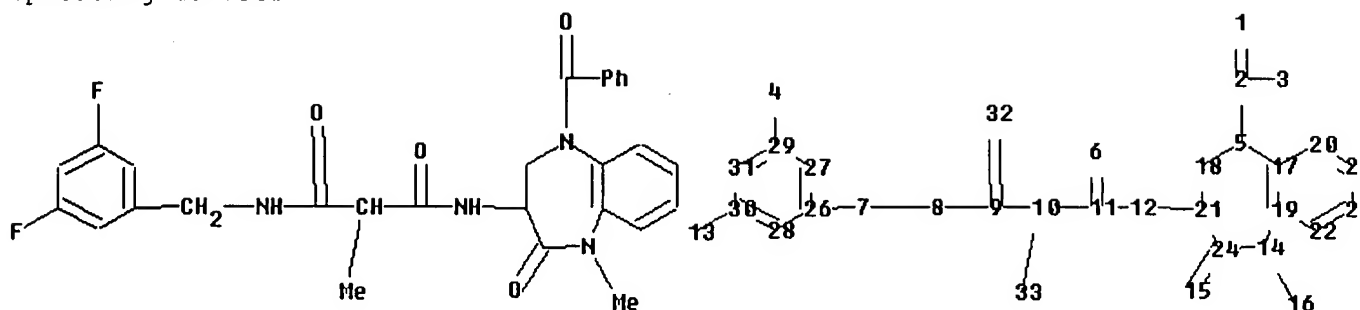
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G3: [*6], [*7]
```

```

Connectivity :
44:2 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:Atom
31:CLASS 32:CLASS 33:Atom 43:CLASS 44:CLASS

```

Uploading L34.str



chain nodes :

1 2 3 4 6 7 8 9 10 11 12 13 15 16 32 33

ring nodes :

5 14 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31

chain bonds :

1-2 2-5 2-3 4-29 6-11 7-8 7-26 8-9 9-10 9-32 10-11 10-33 11-12 12-21
13-30 14-16 15-24

ring bonds :

5-17 5-18 14-19 14-24 17-19 17-20 18-21 19-22 20-23 21-24 22-25 23-25
26-27 26-28 27-29 28-30 29-31 30-31

exact/norm bonds :

1-2 2-5 5-17 5-18 6-11 8-9 9-32 11-12 12-21 14-19 14-24 15-24 18-21
21-24

exact bonds :

2-3 4-29 7-8 7-26 9-10 10-11 10-33 13-30 14-16

normalized bonds :

17-19 17-20 19-22 20-23 22-25 23-25 26-27 26-28 27-29 28-30 29-31 30-31

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:Atom 15:CLASS 16:CLASS 17:Atom 18:Atom

19:Atom 20:Atom

21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom

30:Atom 31:Atom

32:CLASS 33:CLASS

=> d ide L33

L33 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 741672-69-5 REGISTRY

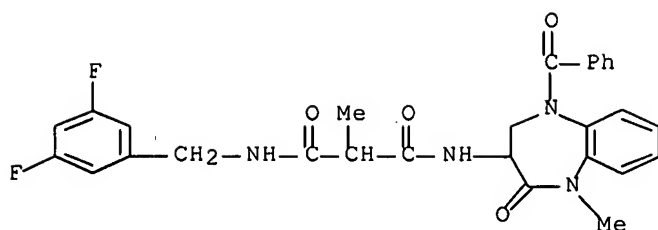
ED Entered STN: 09 Sep 2004

CN **Propanediamide, N-(5-benzoyl-2,3,4,5-tetrahydro-1-methyl-2-oxo-1H-1,5-benzodiazepin-3-yl)-N'-[(3,5-difluorophenyl)methyl]-2-methyl- (9CI)**
(CA INDEX NAME)

MF C28 H26 F2 N4 O4

SR CA

LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> => file marpat

FILE 'MARPAT' ENTERED AT 13:57:06 ON 02 MAY 2007

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FILE CONTENT: 1961-PRESENT VOL 146 ISS 18 (20070427/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

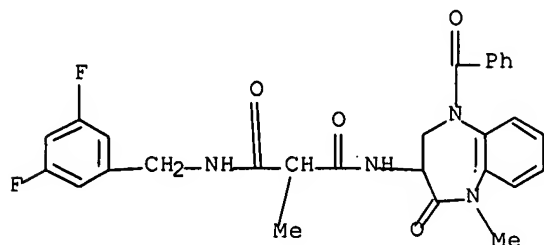
MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2007060644	15 MAR 2007
DE	102006023116	15 MAR 2007
EP	1762248	14 MAR 2007
JP	2007059877	08 MAR 2007
WO	2007030662	15 MAR 2007
GB	2429975	14 MAR 2007
FR	2890657	16 MAR 2007
RU	2295953	27 MAR 2007
CA	2556850	24 FEB 2007

Expanded G-group definition display now available.

=> d stat que L38

L34 STR



Structure attributes must be viewed using STN Express query preparation.

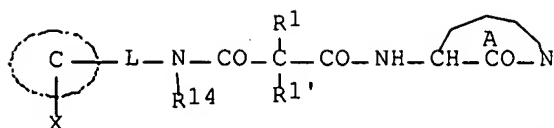
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L38 1 SEA FILE=MARPAT ABB=ON PLU=ON L37/COM

=> d ibib abs qhit L38 1

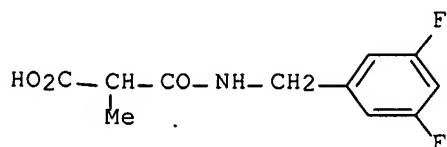
L38 ANSWER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:206827 MARPAT Full-text
TITLE: Preparation of malonamides and related compounds as
gamma-secretase inhibitors for the treatment of
Alzheimer's disease.
INVENTOR(S): Galley, Guido; Goergler, Annick; Jacobsen, Helmut;
Kitas, Eric Argirios; Peters, Jens-Uwe
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069826	A1	20040819	WO 2004-EP674	20040127
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004210036	A1	20040819	AU 2004-210036	20040127
CA 2514267	A1	20040819	CA 2004-2514267	20040127
EP 1592684	A1	20051109	EP 2004-705404	20040127
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BR 2004007262	A	20060131	BR 2004-7262	20040127
CN 1745076	A	20060308	CN 2004-80003305	20040127
JP 2006516556	T	20060706	JP 2006-500017	20040127
US 2004220222	A1	20041104	US 2004-767784	20040129
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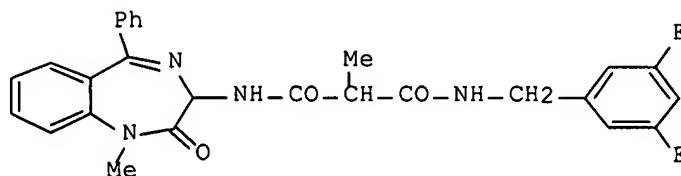
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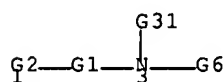
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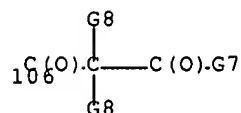
III

AB Title compds. I [L = bond, (CH₂)₁₋₂, CH(CH₃), etc.; C = cyclic ring, e.g., Ph, pyridinyl, furanyl, etc.; X = (R₂)_{1,2,3}; (R₂)_{1,2,3} = H, OH, halo, etc.; R₁, R_{1'} = H, alkyl, halo, etc.; R₁₄ = H, alkyl, (CH₂)₂OH, etc.; A = substituted 5,7-dihydro-6H-dibenz[b,d]azepin-6-ones, 1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-ones, 3,4-dihydro-2-quinolinones, etc.] and their pharmaceutically acceptable salts and formulations were prepared. For example, coupling of 3-amino-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one and malonic acid II, e.g., prepared from di-Et Me malonate in 3-steps, afforded malonamide III in 67% yield. In γ -secretase inhibition assays, 37-examples of compds. I exhibited IC₅₀ values ranging from 0.003-0.11 μ M, the IC₅₀ value of malonamide III was 0.83 μ M. Compds. I are claimed useful for the treatment of Alzheimer's disease.

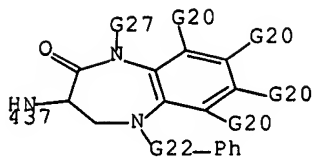
MSTR 1



G₁ = CH₂
G₂ = Ph (opt. substd. by (1-3) G₃)
G₃ = F
G₆ = 106



G7 = 437



G8 = alkyl <containing 1-6 C>

G22 = C(O)

G27 = Me

Patent location: claim 1

Note: and pharmaceutically suitable acid addition salts

Note: also incorporates claim 16

Note: substitution is restricted

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DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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=> file caplus

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PCL XL error

Subsystem: USERSTREAM

Error: MissingData

Operator: 0x0

Position: 0

PCL XL error

Subsystem: KERNEL

Error: StreamUndefined

Operator: 0x0

Position: 0

10/767784.

=> file registry

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DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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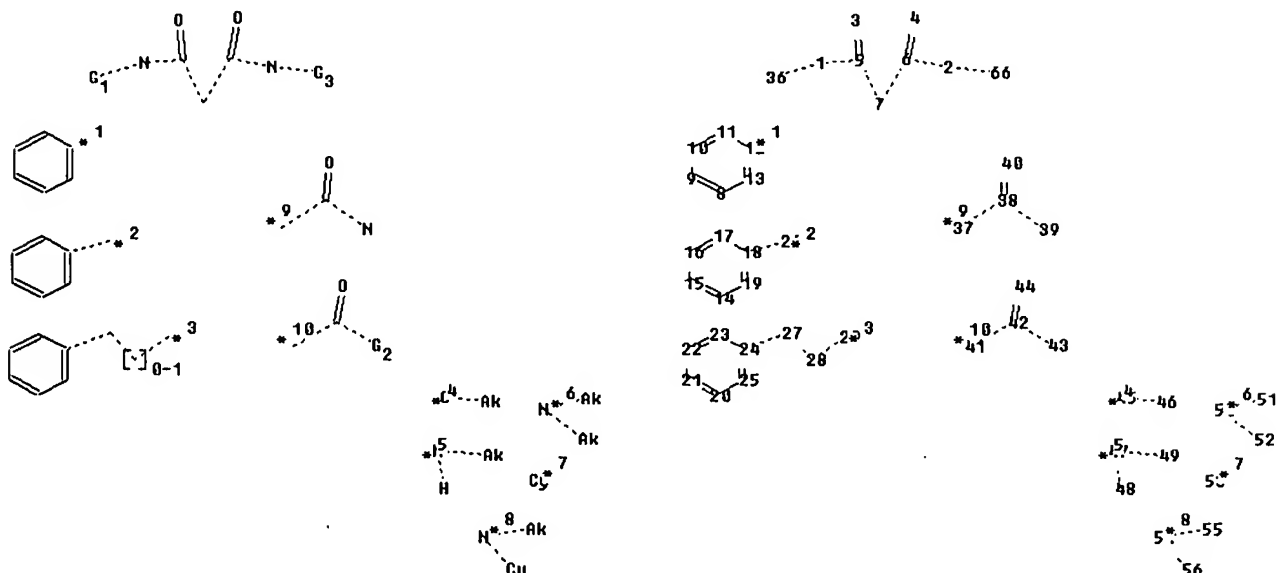
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54 55 56 66

ring nodes :

8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 37 38 39

ring/chain nodes :

```

26 27 28 29
chain bonds :
1-5 1-36 2-6 2-66 3-5 4-6 5-7 6-7 18-26 24-27 38-40 41-42 42-43 42-44
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27-28 28-29
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20-25 21-22 22-23 23-24 24-25 37-38 38-39
exact/norm bonds :
1-5 1-36 2-6 2-66 3-5 4-6 5-7 6-7 18-26 24-27 27-28 28-29 37-38 38-39
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8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17 17-18 18-19 20-
21
20-25 21-22 22-23 23-24 24-25

```

G1: [*1], [*2], [*3]

G2: [*4], [*5], [*6], [*7], [*8]

G3: [*9], [*10]

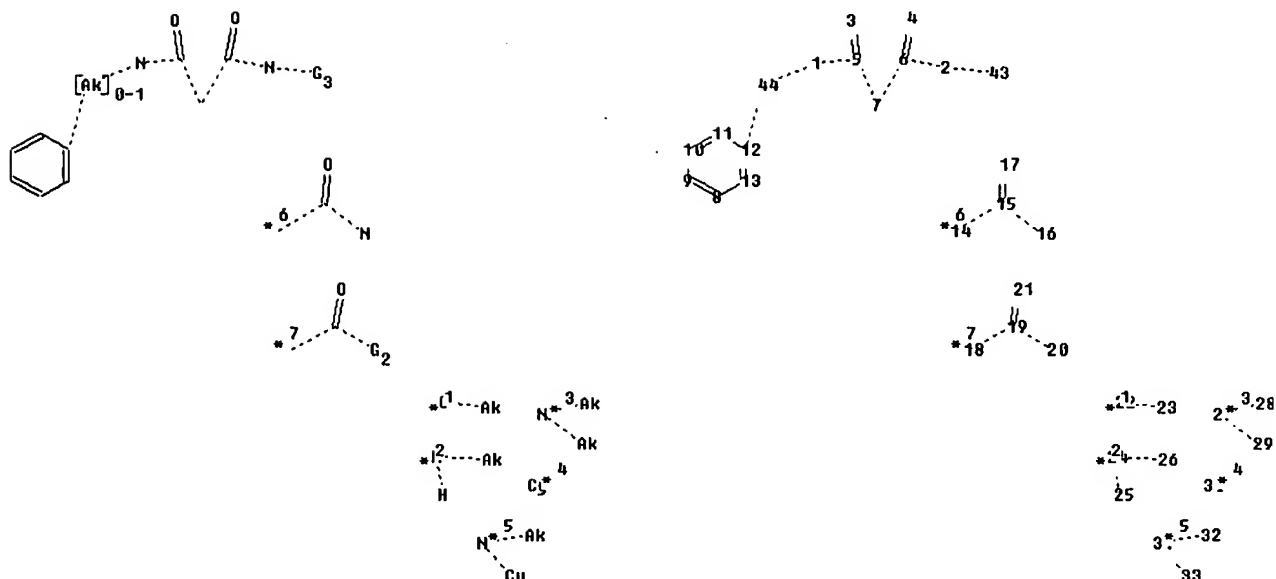
Match level :

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1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS 29:CLASS
36:CLASS 37:Atom
38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS
46:CLASS 47:CLASS
48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:Atom 54:CLASS 55:CLASS
56:Atom 66:CLASS

```

Uploading L9.str



chain nodes :

1 2 3 4 5 6 7 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
32 33 43 44

ring nodes :

8 9 10 11 12 13 14 15 16

chain bonds :

1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 15-17 18-19 19-20 19-21 22-23
24-25 24-26 27-28 27-29 31-32 31-33

ring bonds :

8-9 8-13 9-10 10-11 11-12 12-13 14-15 15-16

exact/norm bonds :

1-5 1-44 2-6 2-43 3-5 4-6 5-7 6-7 12-44 14-15 15-16 15-17 18-19 19-20
19-21 22-23 24-25 24-26 27-28 27-29 31-32 31-33

normalized bonds :

8-9 8-13 9-10 10-11 11-12 12-13

isolated ring systems :

containing 8 :

G2: [*1], [*2], [*3], [*4], [*5]

G3: [*6], [*7]

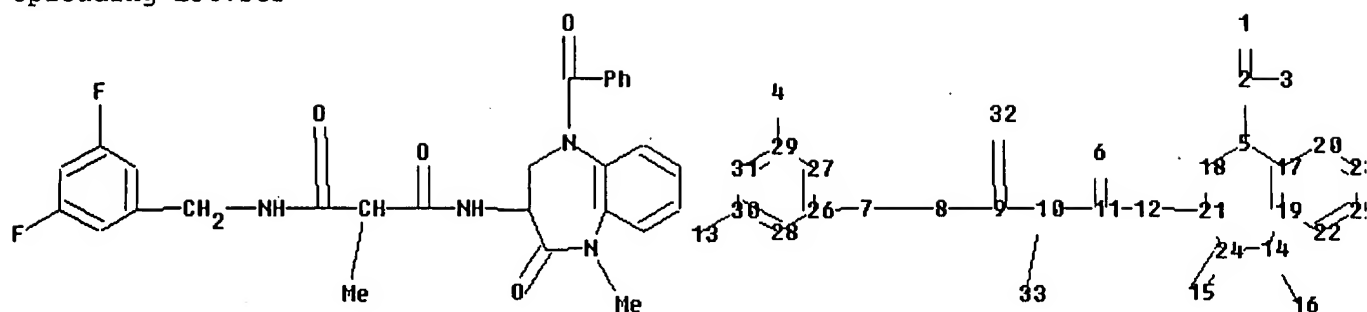
Connectivity :

44:2 E exact RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:Atom
31:CLASS 32:CLASS 33:Atom 43:CLASS 44:CLASS

Uploading L34.str



chain nodes :

1 2 3 4 6 7 8 9 10 11 12 13 15 16 32 33

ring nodes :

5 14 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31

chain bonds :

1-2 2-5 2-3 4-29 6-11 7-8 7-26 8-9 9-10 9-32 10-11 10-33 11-12 12-21
13-30 14-16 15-24

ring bonds :

5-17 5-18 14-19 14-24 17-19 17-20 18-21 19-22 20-23 21-24 22-25 23-25
26-27 26-28 27-29 28-30 29-31 30-31

exact/norm bonds :

1-2 2-5 5-17 5-18 6-11 8-9 9-32 11-12 12-21 14-19 14-24 15-24 18-21
21-24

exact bonds :

2-3 4-29 7-8 7-26 9-10 10-11 10-33 13-30 14-16

normalized bonds :

17-19 17-20 19-22 20-23 22-25 23-25 26-27 26-28 27-29 28-30 29-31 30-31

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:Atom 15:CLASS 16:CLASS 17:Atom 18:Atom

19:Atom 20:Atom

21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom

30:Atom 31:Atom

32:CLASS 33:CLASS

=> d ide L33

L33 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 741672-69-5 REGISTRY

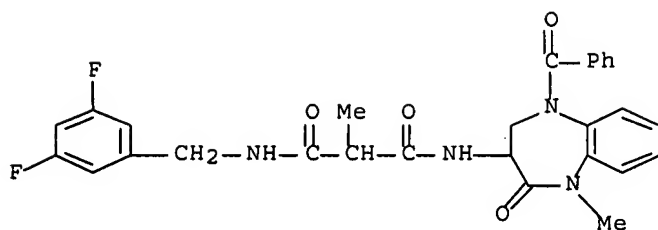
ED Entered STN: 09 Sep 2004

CN Propanediamide, N-(5-benzoyl-2,3,4,5-tetrahydro-1-methyl-2-oxo-1H-1,5-benzodiazepin-3-yl)-N'-[(3,5-difluorophenyl)methyl]-2-methyl- (9CI)
(CA INDEX NAME)

MF C28 H26 F2 N4 O4

SR CA

LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> => file marpat

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FILE CONTENT: 1961-PRESENT VOL 146 ISS 18 (20070427/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

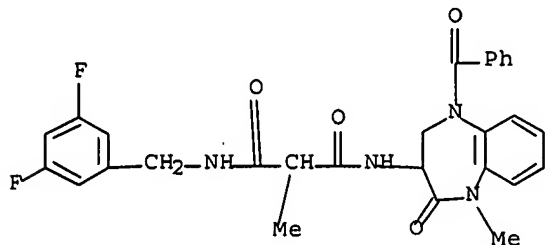
MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2007060644	15	MAR	2007
DE	102006023116	15	MAR	2007
EP	1762248	14	MAR	2007
JP	2007059877	08	MAR	2007
WO	2007030662	15	MAR	2007
GB	2429975	14	MAR	2007
FR	2890657	16	MAR	2007
RU	2295953	27	MAR	2007
CA	2556850	24	FEB	2007

Expanded G-group definition display now available.

=> d stat que L38

L34 STR



Structure attributes must be viewed using STN Express query preparation.

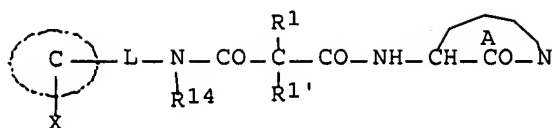
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L38 1 SEA FILE=MARPAT ABB=ON PLU=ON L37/COM

=> d ibib abs qhit L38 1

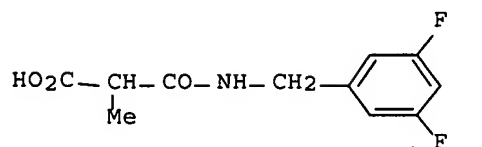
L38 ANSWER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:206827 MARPAT Full-text
TITLE: Preparation of malonamides and related compounds as
gamma-secretase inhibitors for the treatment of
Alzheimer's disease.
INVENTOR(S): Galley, Guido; Goergler, Annick; Jacobsen, Helmut;
Kitas, Eric Argirios; Peters, Jens-Uwe
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069826	A1	20040819	WO 2004-EP674	20040127
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				CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
				GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
				LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
RW:				BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
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				GQ, GW, ML, MR, NE, SN, TD, TG
AU 2004210036	A1	20040819	AU 2004-210036	20040127
CA 2514267	A1	20040819	CA 2004-2514267	20040127
EP 1592684	A1	20051109	EP 2004-705404	20040127
R:				AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
				IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
BR 2004007262	A	20060131	BR 2004-7262	20040127
CN 1745076	A	20060308	CN 2004-80003305	20040127
JP 2006516556	T	20060706	JP 2006-500017	20040127
US 2004220222	A1	20041104	US 2004-767784	20040129
NO 2005003627	A	20050810	NO 2005-3627	20050726
PRIORITY APPLN. INFO.:			EP 2003-2190	20030204
			WO 2004-EP674	20040127

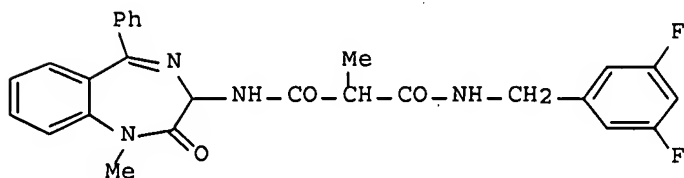
GI



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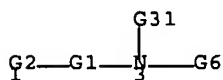
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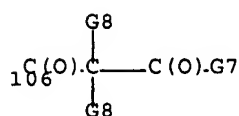
III

AB Title compds. I [L = bond, (CH₂)₁₋₂, CH(CH₃), etc.; C = cyclic ring, e.g., Ph, pyridinyl, furanyl, etc.; X = (R₂)_{1,2,3}; (R₂)_{1,2,3} = H, OH, halo, etc.; R₁, R_{1'} = H, alkyl, halo, etc.; R₁₄ = H, alkyl, (CH₂)₂OH, etc.; A = substituted 5,7-dihydro-6H-dibenz[b,d]azepin-6-ones, 1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-ones, 3,4-dihydro-2-quinolinones, etc.] and their pharmaceutically acceptable salts and formulations were prepared. For example, coupling of 3-amino-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one and malonic acid II, e.g., prepared from di-Et Me malonate in 3-steps, afforded malonamide III in 67% yield. In γ -secretase inhibition assays, 37-examples of compds. I exhibited IC₅₀ values ranging from 0.003-0.11 μ M, the IC₅₀ value of malonamide III was 0.83 μ M. Compds. I are claimed useful for the treatment of Alzheimer's disease.

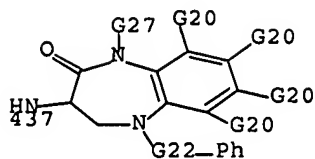
MSTR 1



G1 = CH₂
G2 = Ph (opt. substd. by (1-3) G3)
G3 = F
G6 = 106



G7 = 437



G8 = alkyl <containing 1-6 C>

G22 = C(O)

G27 = Me

Patent location: claim 1

Note: and pharmaceutically suitable acid addition salts

Note: also incorporates claim 16

Note: substitution is restricted

=> => file registry

FILE 'REGISTRY' ENTERED AT 14:00:33 ON 02 MAY 2007

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STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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FILE LAST UPDATED: 1 May 2007 (20070501/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L16

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L16 1 SEA FILE=CAPLUS ABB=ON PLU=ON L15

=> d stat que L48

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L40 4 SEA FILE=CAPLUS ABB=ON PLU=ON GOERGLER A?/AU
L41 297 SEA FILE=CAPLUS ABB=ON PLU=ON JACOBSEN H?/AU
L42 45 SEA FILE=CAPLUS ABB=ON PLU=ON KITAS E?/AU
L43 2834 SEA FILE=CAPLUS ABB=ON PLU=ON PETERS J?/AU
L44 9 SEA FILE=CAPLUS ABB=ON PLU=ON L39 AND (L40 OR L41 OR L42 OR L43)
L45 1 SEA FILE=CAPLUS ABB=ON PLU=ON L40 AND (L41 OR L42 OR L43)
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L48 9 SEA FILE=CAPLUS ABB=ON PLU=ON (L44 OR L45 OR L46 OR L47)

=> d stat que L49
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L3 527 SEA FILE=REGISTRY SSS FUL L1
L7 4 SEA FILE=REGISTRY ABB=ON PLU=ON L3 AND C3/ESS
L8 3 SEA FILE=CAPLUS ABB=ON PLU=ON L7
L9 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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L24 1 SEA FILE=REGISTRY ABB=ON PLU=ON 146420-49-7
L25 369 SEA FILE=REGISTRY ABB=ON PLU=ON L12 NOT L24
L26 65 SEA FILE=CAPLUS ABB=ON PLU=ON L25
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L40 4 SEA FILE=CAPLUS ABB=ON PLU=ON GOERGLER A?/AU
L41 297 SEA FILE=CAPLUS ABB=ON PLU=ON JACOBSEN H?/AU
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L43) AND (L8 OR L26)

=> s (L16 or L48-L49)
L50 9 (L16 OR (L48 OR L49))

=> d ibib abs hitind L50 1-9

L50 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:175657 CAPLUS Full-text
DOCUMENT NUMBER: 146:251750
TITLE: Preparation of fluoro substituted 2-oxo-azepan
derivatives as γ -secretase inhibitors
INVENTOR(S): Flohr, Alexander; Galley, Guido;
Jakob-Roetne, Roland; Kitas, Eric Argirios;
Wostl, Wolfgang
PATENT ASSIGNEE(S): Switz.
SOURCE: U.S. Pat. Appl. Publ., 18pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2007037789	A1	20070215	US 2006-500662	20060808
WO 2007020190	A1	20070222	WO 2006-EP64935	20060802
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
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IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:

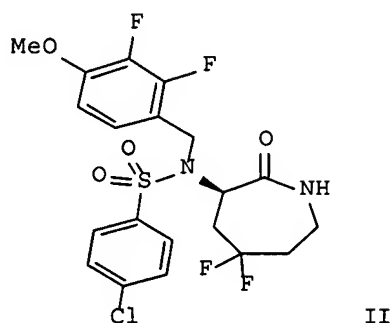
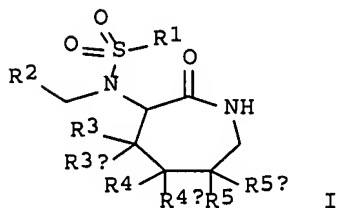
EP 2005-107455

A 20050812

OTHER SOURCE(S):

MARPAT 146:251750

GI



AB The title fluoro substituted 2-oxo-azepan derivs. I [wherein R1 = halogenated alkyl or (un)substituted (hetero)aryl; R2 = (un)substituted heterocycloalkyl or (hetero)aryl; R3/R3a, R4/R4a, and R5/R5a = independently H or F; wherein at least one of R4/R4a and R5/R5a = F], or pharmaceutically acceptable acid salts, optical enantiomers, racemates, or diastereomeric mixts. thereof were prepared as γ -secretase inhibitors for the treatment of Alzheimer's disease or common cancers including, but not limited to, cervical carcinomas, breast carcinomas, and malignancies of the hematopoietic system (no data). For example, 4-chloro-N-((R)-5,5-difluoro-2-oxo-azepan-3-yl)benzenesulfonamide (preparation given) was alkylated using 1-bromomethyl-2,3-difluoro-4-methoxybenzene to give II. II showed inhibitory activity with IC50 of 2 nM against γ -secretase. Formulations as tablets and capsules were described.

INCL 514212030; 540527000

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

L50 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:53048 CAPLUS Full-text

DOCUMENT NUMBER: 144:128869

TITLE: Preparation of N-(2-oxoazepan-3-yl)sulfonamides as γ -secretase inhibitors for treating Alzheimer's disease and cancers

INVENTOR(S): Galley, Guido; Kitas, Eric, Argirios
; Jakob-Roetne, Roland

PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.

SOURCE: PCT Int. Appl., 107 pp.

CODEN: PIXXD2

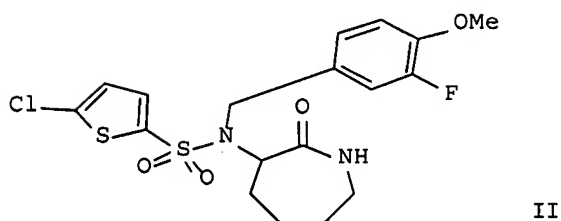
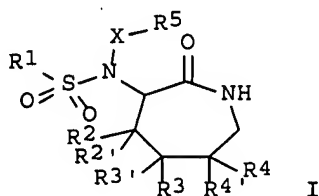
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006005486	A1	20060119	WO 2005-EP7268	20050706
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005261932	A1	20060119	AU 2005-261932	20050706
CA 2573372	A1	20060119	CA 2005-2573372	20050706
EP 1768960	A1	20070404	EP 2005-754795	20050706
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
US 2006014945	A1	20060119	US 2005-179703	20050712
PRIORITY APPLN. INFO.:			EP 2004-103339	A 20040713
			WO 2005-EP7268	W 20050706
OTHER SOURCE(S):		MARPAT 144:128869		
GI				



AB Title compds. I [R1 = (un)substituted hetero/aryl; R2-R4, R2'-R4' = H, lower alkyl, Ph or lower alkyl substituted by halogen; R5 = cycloalkyl, (un)substituted hetero/aryl; X = CHR; R = H, lower alkyl; and their pharmaceutically suitable acid addition salts, optical pure enantiomers, racemates or diastereomeric] were prepared as γ -secretase inhibitors. Thus, reductive amination of 3-fluoro-p-anisaldehyde with 3-aminoazepan-2-one and reaction with 5-chlorothiophene-2-sulfonyl chloride gave sulfonamide II. Preferred I inhibited γ -secretase with $IC_{50} < 0.3 \mu M$. I are useful in the treatment of Alzheimer's disease or common cancers.

IC ICM C07D223-08

ICS A61K031-55; A61P035-00; A61P025-28
 CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1, 63
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:303395 CAPLUS Full-text
 DOCUMENT NUMBER: 142:373708
 TITLE: Preparation of carbamic acid alkyl ester derivatives
 as
 INVENTOR(S): Flohr, Alexander; Galley, Guido;
 Jakob-Roetne, Roland; Kitas, Eric Argirios;
 Peters, Jens-Uwe; Wostl, Wolfgang
 PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 38 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005075327	A1	20050407	US 2004-951229	20040927
US 7166587	B2	20070123		
AU 2004283803	A1	20050506	AU 2004-283803	20040927
CA 2541470	A1	20050506	CA 2004-2541470	20040927
WO 2005040126	A1	20050506	WO 2004-EP10821	20040927
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EP 1673347	A1	20060628	EP 2004-787028	20040927
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BR 2004015070	A	20061212	BR 2004-15070	20040927
CN 1894217	A	20070110	CN 2004-80033374	20040927
JP 2007507447	T	20070329	JP 2006-530028	20040927
NO 2006001469	A	20060626	NO 2006-1469	20060331
PRIORITY APPLN. INFO.:			EP 2003-22650	A 20031006
			WO 2004-EP10821	W 20040927
OTHER SOURCE(S):			CASREACT 142:373708; MARPAT 142:373708	
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The compds. of general formula (I) and (II) [R1 = each (un)substituted - (CHR')q-aryl or -(CHR')q-heteroaryl, lower alkyl, lower alkenyl, -(CH2)nSiMe3, -(CH2)n-O-lower alkyl, -(CH2)n-S-lower alkyl, -(CH2)q-cycloalkyl, or -(CH2)n-

[CH(OH)]_m-(CF₂)_p-CHF(3-q), -(CH₂)_n-CR₂-CF₃ (wherein the two R radicals form together with the carbon atom a cycloalkyl ring); R' = H, lower alkyl; n = 1-3; m = 0, 1; p = 0-6; q = 0-3; R₂ = H, lower alkyl; R₃ = H, lower alkyl, -CH₂CF₂CF₃, CH₂CF₃, (CH₂)₂CF₃, CF₃, CHF₂, CH₂F, (un)substituted aryl, -(CH₂)_nNR₅R₆ (wherein R₅, R₆ = H, lower alkyl); R₄ = Q, Q₁ (wherein R₇ = H, lower alkyl, -(CH₂)_nCF₃, -(CH₂)_n-cycloalkyl); R₈ = H, lower alkyl, -COPh, -C(O)-lower alkyl, -C(O)O-(CH₂)_n-cycloalkyl, -C(O)O-(CH₂)_n-lower alkyl, -C(O)NH-(CH₂)_n-lower alkyl, -C(O)NH-(CH₂)_n-cycloalkyl; R₉ = H, lower alkyl, -(CH₂)_n-cycloalkyl, -(CH₂)_n-CF₃] or pharmaceutically acceptable salts, optically pure enantiomers, racemates or diastereomeric mixts. thereof are prepared These compds. inhibit amyloidogenic Abeta peptides, i.e. β-amyloid (Aβ) peptides, and are useful for the treatment of Alzheimer's disease. β-amyloid peptides. Thus, 0.12 g (0.25 mmol) carbonic acid 4-nitrophenyl ester (S)-1-((S)-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-ylcarbamoylethyl ester and 543 μl 2,2,3,3,3-pentafluoropropylamine were stirred at room temperature over night to give, after silica gel chromatog., 0.075 g (63%) (2,2,3,3,3-pentafluoropropyl)carbamic acid (1S)-1-(((7S)-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)carbamoylethyl ester (III). III showed IC₅₀ of 0.001 μM against γ-secretase.

IC ICM A61K031-5513

ICS A61K031-55; C07D243-24

INCL 514212040; X51-422.1; X54-050.8; X54-052.2

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 28

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:220131 CAPLUS Full-text

DOCUMENT NUMBER: 142:298014

TITLE: Preparation of dibenzoazepinylmalonamides, dibenzoxepinylmalonamides, benzodiazepinylmalonamides, and related compounds as γ-secretase inhibitors for treatment of Alzheimer's disease.

INVENTOR(S): Flohr, Alexander; Galley, Guido; Jakob-Roetne, Roland; Kitas, Eric Argirios; Peters, Jens-Uwe; Wostl, Wolfgang

PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 59 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

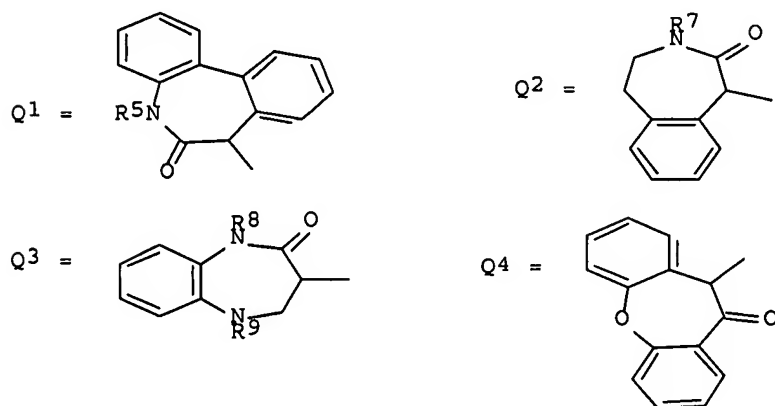
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2005054633	A1	20050310	US 2004-933177	20040902
US 7160875	B2	20070109		
AU 2004270361	A1	20050317	AU 2004-270361	20040831
CA 2537440	A1	20050317	CA 2004-2537440	20040831
WO 2005023772	A1	20050317	WO 2004-EP9700	20040831
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG

BR 2004013533	A	20061010	BR 2004-13533	20040831
EP 1711470	A1	20061018	EP 2004-764665	20040831
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1875005	A	20061206	CN 2004-80032641	20040831
JP 2007505063	T	20070308	JP 2006-525701	20040831
NO 2006001047	A	20060404	NO 2006-1047	20060303
PRIORITY APPLN. INFO.:			EP 2003-19683	A 20030909
			WO 2004-EP9700	W 20040831

OTHER SOURCE(S): MARPAT 142:298014
 GI



AB Malonamides R1NHCOCR3R4CONHR2 [R1= Q1-Q4; R2 = alkyl, alkynyl, alkylthio, alkoxy(alkyl), halo(alkyl), etc.; R3, R4 = H, alkyl, alkoxy, Ph, halo; R5 = H, alkyl, trifluoromethyl(alkyl), cycloalkyl(alkyl); R6 = H, halo; R7 = H, alkyl; R8 = H, alkyl, alkynyl, trifluoromethyl(alkyl), cycloalkyl(alkyl), (halo-substituted) phenyl(alkyl); R9 = H, alkyl, CHO, alkylcarbonyl, F3CCO, (substituted) PhCO, etc.], were prepared. Thus, 2-methyl-N-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)malonamic acid (preparation given), cyclopropylmethylamine, and 2-(2-pyridon-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate (TPTU) were shaken together overnight in DMF to give N-cyclopropylmethyl-2-methyl-N'-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)malonamide. The latter inhibited γ -secretase with IC50 = 0.09 μ M.

IC ICM A61K031-55

ICS A61K031-5513; A61K031-335

INCL 514212040; X51-421.207; X51-422.1; X51-445.0; X54-050.9; X54-052.2; X54-052.3

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 28, 63

IT	847927-01-9P	847927-02-0P	847927-03-1P	847927-04-2P	847927-05-3P
	847927-06-4P	847927-07-5P	847927-08-6P	847927-09-7P	847927-10-0P
	847927-11-1P	847927-12-2P	847927-13-3P	847927-14-4P	

847927-15-5P	847927-16-6P	847927-17-7P	847927-18-8P	847927-19-9P
847927-20-2P	847927-21-3P	847927-22-4P	847927-23-5P	847927-24-6P
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847927-35-9P	847927-36-0P	847927-37-1P	847927-47-3P	847927-50-8P
847927-51-9P	847927-52-0P	847927-53-1P	847927-54-2P	847927-55-3P
847927-56-4P	847927-57-5P	847927-58-6P	847927-59-7P	847927-60-0P
847927-61-1P	847927-62-2P	847927-63-3P	847927-64-4P	847927-65-5P
847927-66-6P	847927-67-7P	847927-68-8P	847927-69-9P	847927-70-2P
847927-71-3P	847927-72-4P	847927-73-5P	847927-74-6P	

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dibenzoazepinylmalonamides, dibenzooxepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ -secretase inhibitors for treatment of Alzheimer's disease)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1019771 CAPLUS Full-text

DOCUMENT NUMBER: 142:6564

TITLE: Preparation of 1,4-benzoxazepin-3-ones as inhibitors of γ -secretase for the treatment of Alzheimer's disease

INVENTOR(S): Galley, Guido; Goodnow, Robert Alan; Peters, Jens-Uwe

PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 27 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2004235819	A1	20041125	US 2004-838054	20040503
US 7060698	B2	20060613		
AU 2004238037	A1	20041125	AU 2004-238037	20040514
CA 2524640	A1	20041125	CA 2004-2524640	20040514
WO 2004100958	A1	20041125	WO 2004-EP5177	20040514
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1631296	A1	20060308	EP 2004-732944	20040514
EP 1631296	B1	20070425		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1794997	A	20060628	CN 2004-80014015	20040514
BR 2004010647	A	20060704	BR 2004-10647	20040514
JP 2007501261	T	20070125	JP 2006-529815	20040514

PRIORITY APPLN. INFO.:

EP 2003-11040

A 20030519

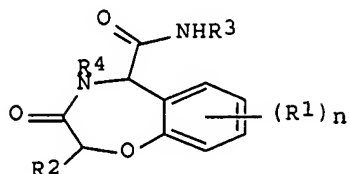
WO 2004-EP5177

W 20040514

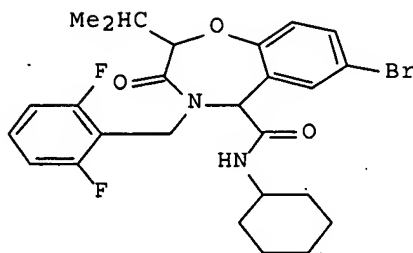
OTHER SOURCE(S):

MARPAT 142:6564

GI



I



II

AB 1,4-Benzooxazepin-3-ones I [m = 0-2; n = 1, 2; p = 1, 2; R1 = H, halogen, alkoxy, amino, alkylamino, dialkylamino; R2 = H, alkyl, cycloalkyl-(CH2)m, Ph(CH2)m, alkoxy-(CH2)m; R3 = alkyl, alkoxycarbonyl-(CH2)m, Ph(CH2)m, cycloalkyl; R4 = (un)substituted Ph(CH2)p, cycloalkyl, tetrahydronaphthalen-1-yl, 9-fluorenyl, alkyl] such as II are prepared as γ -secretase inhibitors for the treatment of Alzheimer's disease. Treatment of 5-bromosalicylaldehyde with base followed by addition of Et 2-bromo-3-methylbutyrate yields Et 2-(4-bromo-2-formylphenoxy)-3-methylbutanoate, which is hydrolyzed to yield 2-(4-bromo-2-formylphenoxy)-3-methylbutanoic acid (III); stirring III with 2,6-difluorobenzylamine and cyclohexyl isocyanide in DMSO yields II. IC50 values (without units) are given for the inhibition of γ -secretase by some of the title compds. E.g., II inhibits γ -secretase with an IC50 value of 0.28 (no units given). A process for the preparation of the title compds. using a cyclocondensation of (formylaryloxy)alkanoic acids, amines, and isonitriles is claimed.

IC ICM A61K031-553

ICS C07D413-02

INCL 514211050; X54-049.0

CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:675740 CAPLUS Full-text

DOCUMENT NUMBER: 141:206827

TITLE: Preparation of malonamides and related compounds as γ -secretase inhibitors for the treatment of Alzheimer's disease.

INVENTOR(S): Galley, Guido; Goergler, Annick; Jacobsen, Helmut; Kitas, Eric Argirios; Peters, Jens-Uwe

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

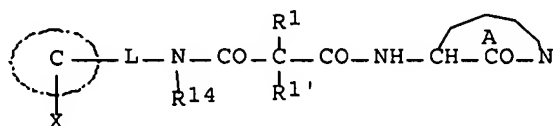
DOCUMENT TYPE: Patent

LANGUAGE: English

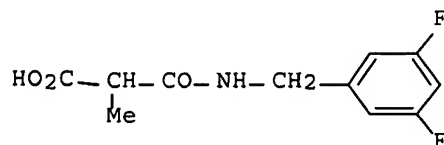
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

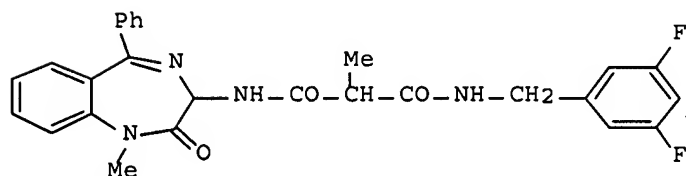
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069826	A1	20040819	WO 2004-EP674	20040127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004210036	A1	20040819	AU 2004-210036	20040127
CA 2514267	A1	20040819	CA 2004-2514267	20040127
EP 1592684	A1	20051109	EP 2004-705404	20040127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004007262	A	20060131	BR 2004-7262	20040127
CN 1745076	A	20060308	CN 2004-80003305	20040127
JP 2006516556	T	20060706	JP 2006-500017	20040127
US 2004220222	A1	20041104	US 2004-767784	20040129
NO 2005003627	A	20050810	NO 2005-3627	20050726
PRIORITY APPLN. INFO.:			EP 2003-2190	A 20030204
			WO 2004-EP674	W 20040127
OTHER SOURCE(S):		MARPAT 141:206827		
GI				



I



II



III

AB Title compds. I [L = bond, (CH₂)₁₋₂, CH(CH₃), etc.; C = cyclic ring, e.g., Ph, pyridinyl, furanyl, etc.; X = (R₂)_{1,2,3}; (R₂)_{1,2,3} = H, OH, halo, etc.; R₁, R₁' = H, alkyl, halo, etc.; R₁₄ = H, alkyl, (CH₂)₂OH, etc.; A = substituted 5,7-dihydro-6H-dibenz[b,d]azepin-6-ones, 1,3-dihydro-5-phenyl- 1,4-benzodiazepin-2-ones, 3,4-dihydro-2-quinolinones, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, coupling of 3-amino-1,3-dihydro-1-methyl-5-phenyl-2H-1,4- benzodiazepin-2-one and malonamic acid II, e.g., prepared from di-Et Me malonate in 3-steps, afforded malonamide III in 67% yield. In γ -secretase inhibition assays, 37-

examples of compds. I exhibited IC50 values ranging from 0.003-0.11 μ M, the IC50 value of malonamide III was 0.83 μ M. Compds. I are claimed useful for the treatment of Alzheimer's disease.

IC ICM C07D401-06
ICS C07D217-06; C07D403-06; C07D471-08; C07D401-04; C07D471-04;
C07D471-06; C07D209-44; C07D209-18; C07D223-18; C07D401-12;
C07D405-12; C07D409-12; C07C237-12; C07C237-14

CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 1, 63

IT 741672-55-9P 741672-56-0P 741672-57-1P
741672-58-2P 741672-59-3P 741672-60-6P
741672-61-7P 741672-62-8P 741672-63-9P
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741672-95-7P 741672-96-8P 741672-97-9P
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 741674-40-8P 741674-99-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of malonamides and related compds. as γ -secretase
 inhibitors for the treatment of Alzheimer's disease.)

IT 2985-33-3P, 2-Methylmalonic acid monoethyl ester 119860-05-8P
 741674-41-9P 741674-42-0P 741674-44-2P 741674-45-3P 741674-46-4P
 741674-47-5P 741674-48-6P 741674-49-7P 741674-50-0P
 741674-51-1P 741674-54-4P 741674-55-5P 741674-56-6P 741674-57-7P
 741674-58-8P 741674-59-9P, N-(3,5-Difluorobenzyl)malonamic acid
 741674-60-2P 741674-64-6P 741674-65-7P 741674-66-8P 741674-67-9P
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 741674-73-7P 741674-74-8P 741674-75-9P 741674-78-2P 741674-79-3P
 741674-81-7P 741674-82-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation of malonamides and related compds. as γ -secretase
 inhibitors for the treatment of Alzheimer's disease.)

L50 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:888744 CAPLUS Full-text
 DOCUMENT NUMBER: 137:384847
 TITLE: 1-Oxa-3,9-diazaspiro[5,5]undecan-2-ones as antagonists
 of the neurokinin receptor
 INVENTOR(S): Cai, Hai-Ying; Dillon, Michael Patrick; Galley,
 Guido; Goergler, Annick; Kolczewski,
 Sabine; Muszynski-Barsy, Dawn Marie
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
 SOURCE: PCT Int. Appl., 36 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

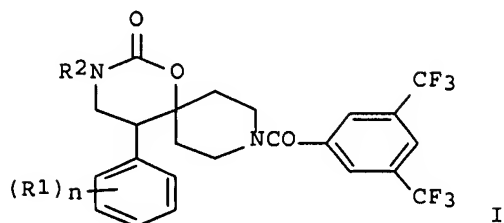
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092604	A1	20021121	WO 2002-EP4935	20020506
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2447329	A1	20021121	CA 2002-2447329	20020506
AU 2002342238	A1	20021125	AU 2002-342238	20020506
EP 1390372	A1	20040225	EP 2002-742943	20020506

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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

BR 2002009604	A	20040323	BR 2002-9604	20020506
CN 1507449	A	20040623	CN 2002-809473	20020506
JP 2004534758	T	20041118	JP 2002-589488	20020506
US 2003004163	A1	20030102	US 2002-143431	20020510
US 6599900	B2	20030729		
ZA 2003008535	A	20050131	ZA 2003-8535	20031031

PRIORITY APPLN. INFO.: EP 2001-111644 A 20010514
 WO 2002-EP4935 W 20020506

OTHER SOURCE(S): MARPAT 137:384847
 GI



AB Title compds. I [R1 = halogen, alkyl, alkoxy; R2 = H, alkyl, haloalkyl, OH, hydroxyalkyl, amino, aminoalkyl, alkoxyalkyl, carbamoylalkyl, heteroaryl, heteroarylalkyl, heterocyclic, heterocyclalkyl; n = 0-2] were prepared for use as NK-1 antagonists. Thus, 3-ClC6H4CH2CN was treated with 1-[3,5-bis(trifluoromethyl)benzoyl]-4-piperidinone and cyclized with carbonyldiimidazole to give I [R1 = 3-Cl, R2 = H] which had a pKi for the NK-1 receptor of 8.29.

IC ICM C07D498-10
 ICS A61K031-535

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:904170 CAPLUS Full-text
 DOCUMENT NUMBER: 136:37519
 TITLE: Synthesis and use of triazaspirodecanone derivatives as neurokinin receptor antagonists
 INVENTOR(S): Galley, Guido; Godel, Thierry; Goergler, Annick; Hoffmann, Torsten; Kolczewski, Sabine; Roevers, Stephan
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.
 SOURCE: PCT Int. Appl., 90 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2001094346      A1      20011213      WO 2001-EP6305      20010601
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    CZ, DE, DK, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
    IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
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US 2002006932      A1      20020117      US 2001-861795      20010521
US 6482829          B2      20021119
CA 2411716          A1      20011213      CA 2001-2411716      20010601
EP 1292596          A1      20030319      EP 2001-945242      20010601
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BR 2001011538      A      20030701      BR 2001-11538      20010601
JP 2003535863      T      20031202      JP 2002-501895      20010601
ZA 2002009488      A      20040223      ZA 2002-9488      20021121
PRIORITY APPLN. INFO.:
                                EP 2000-112285      A 20000608
                                WO 2001-EP6305      W 20010601

OTHER SOURCE(S):      MARPAT 136:37519
GI

```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, alkyl, alkenyl, Ph, (CH₂)_m-non aromatic heterocyclyl, (CH₂)_m-heteroaryl, (CH₂)_m-carboxamide, (CH₂)_m-C(O)alkyl, etc.; R2 = H, alkyl, halo, alkoxy; R3 = alkyl, alkoxy, halo, CF₃; X = N-, C:, CH; X1/X2 = H, OH, alkoxy or may be together an oxo group; Y1/Y2 = H, alkyl, (CH₂)_m-Ph or may be together an oxo group; Z = bond, CH₂, C(O); m = 0 - 4; n = 2 - 3; p = 0 - 2] were prepared Over 160 synthetic examples were disclosed. For example, 8-(3,5-bistrifluoromethylbenzoyl)-1-phenyl-1,3,8- triazaspiro[4.5]decan-4-one was reacted with 2-chloro-4,6-dimethoxy-1,3,5- triazine (1,2-dimethoxyethane, NaH, 100°C, 1 h) to give II. II had pK_i = 8.66 for the NK-1 receptor. I are useful in the treatment of diseases related to NK-1 receptor antagonists.

IC ICM C07D471-10
ICS A61K031-445; C07D471-10; C07D239-00; C07D221-00

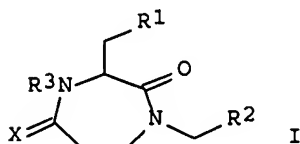
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:868429 CAPLUS Full-text
DOCUMENT NUMBER: 136:6018
TITLE: 1,4-Diazepan-2,5-dione derivatives and their use as NK-1 receptor antagonists
INVENTOR(S): Galley, Guido; Goergler, Annick;
Godel, Thierry; Heck, Reinhard
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090083	A1	20011129	WO 2001-EP5723	20010518
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US 2002010174	A1	20020124	US 2001-854885	20010514
US 6452001	B2	20020917		
CA 2409842	A1	20011129	CA 2001-2409842	20010518
EP 1296961	A1	20030402	EP 2001-960225	20010518
EP 1296961	B1	20070214		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011062	A	20030610	BR 2001-11062	20010518
JP 2003534332	T	20031118	JP 2001-586272	20010518
AT 353881	T	20070315	AT 2001-960225	20010518
ZA 2002008940	A	20040204	ZA 2002-8940	20021104
PRIORITY APPLN. INFO.:			EP 2000-111249	A 20000525
			WO 2001-EP5723	W 20010518
OTHER SOURCE(S):		MARPAT 136:6018		
GI				



AB Title compds. I [R1, R2 = (un)substituted aryl, heteroaryl; R3 = H, alkyl, aminoalkyl, etc.; X = O, alkylimino, aminoalkylimino, etc.] were prepared for treatment of diseases related to the NK-1 receptor. Thus, I [R1 = 3,4-dichlorophenyl, R2 = 3,5-bis(trifluoromethyl)phenyl, R3 = H, X = O] was prepared in 3 steps starting from tert-Bu acrylate and 3,5-bis(trifluoromethyl)benzylamine. The affinities (pKi) of I for the NK-1 receptor were in the 8.00-9.00 range.

IC ICM C07D243-08
 ICS A61K031-551; C07D487-04; A61K031-5517; C07D401-14; C07D403-06; C07D401-06; A61P029-00; A61P025-00; A61P013-10; A61P001-08

CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1, 63

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> file registry

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FILE LAST UPDATED: 1 May 2007 (20070501/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L8

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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L7 4 SEA FILE=REGISTRY ABB=ON PLU=ON L3 AND C3/ESS

L8 3 SEA FILE=CAPLUS ABB=ON PLU=ON L7

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L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L3 527 SEA FILE=REGISTRY SSS FUL L1
L9 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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L24 1 SEA FILE=REGISTRY ABB=ON PLU=ON 146420-49-7
L25 369 SEA FILE=REGISTRY ABB=ON PLU=ON L12 NOT L24
L26 65 SEA FILE=CAPLUS ABB=ON PLU=ON L25

=> s (L8 or L26) not L50
L53 64 (L8 OR L26) NOT L50

=> d ibib abs hitstr L53 1-64

L53 ANSWER 1 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:190950 CAPLUS Full-text
DOCUMENT NUMBER: 146:206636
TITLE: Novel malonic acid derivatives, processes for their
preparation, their use and pharmaceutical compositions
containing them (inhibition of factor Xa activity)
INVENTOR(S): Defossa, Elisabeth; Heinelt, Uwe; Klingler, Otmar;
Zoller, Gerhard; Matter, Hans; Al-Obeidi, Fahad A.;
Walser, Armin; Wildgoose, Peter
PATENT ASSIGNEE(S): Hoechst Marion Roussel Deutschland GmbH, Germany
SOURCE: PCT Int. Appl., 130pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2000040571	A1	20000713	WO 1999-EP10340	19991223
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IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,				
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,				
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,				
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,				
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1016663	A1	20000705	EP 1999-100002	19990102
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IE, SI, LT, LV, FI, RO				
CA 2358578	A1	20000713	CA 1999-2358578	19991223
BR 9916732	A	20010925	BR 1999-16732	19991223
EP 1140878	A1	20011010	EP 1999-964667	19991223
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IE, SI, LT, LV, FI, RO

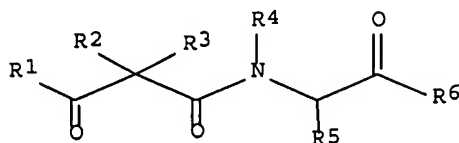
JP 2002534420	T	20021015	JP 2000-592279	19991223
NO 2001002983	A	20010615	NO 2001-2983	20010615
IN 2001CN00908	A	20050304	IN 2001-CN908	20010628

PRIORITY APPLN. INFO.:

EP 1999-100002	A	19990102
EP 1999-119537	A	19991001
WO 1999-EP10340	W	19991223

OTHER SOURCE(S): MARPAT 146:206636

GI



AB The present invention relates to the preparation of new compds. for the inhibition of blood clotting proteins, and more particularly, to malonic acid derivs., I (R1 = organo-amino, organo-alkoxy, etc.; R2 = H, C1-4 alkyl; R3 = (un)substituted C6-10-aryl-C1-4-alkyl; R4 = H, C1-4-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl-C1-4-alkyl; R5 = H, C1-10-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl, C6-10-aryl-C1-4-alkyl, etc.; R4R5 = cyclic hydrocarbyl; R6 = organo-alkoxy, organo-amino, etc.). Thus, 2-(R,S)-(4-carbamimidoylbenzyl)-N-[(S)-cyclohexyl(piperidin-4-yl-carbamoyl)methyl]-N',N'-dimethylmalonamide acetic acid salt was prepared in several steps starting from 2,2-dimethyl[1,3]dioxane-4,6-dione and 4-formyl-benzonitrile. I are inhibitors (Ki = 0.001 - 5.23 μ M) of the blood clotting enzyme factor Xa. The invention also relates to processes for the preparation of I, to methods of inhibiting factor Xa activity and of inhibiting blood clotting, to the use of I in the treatment and prophylaxis of diseases, which can be treated or prevented by the inhibition of factor Xa activity such as thromboembolic diseases, and to the use of the compds. I in the preparation of medicaments to be applied in such diseases.

IT 280553-80-2P 280553-83-5P 280553-85-7P
 280553-87-9P 280553-91-5P 280553-96-0P
 280554-05-4P 280554-33-8P 280554-35-0P
 280554-36-1P 280554-37-2P 923294-55-7P
 923294-56-8P 923294-57-9P 923294-58-0P
 923294-59-1P 923586-00-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of malonic acid derivs. as factor Xa inhibitors and anticoagulant agents)

RN 280553-80-2 CAPLUS

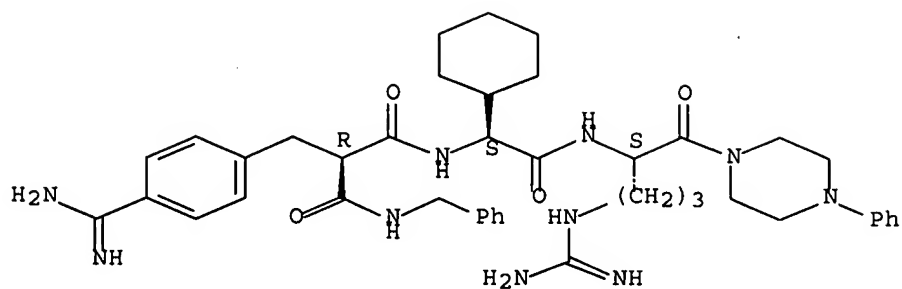
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CRN 280553-79-9

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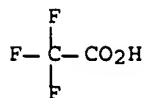
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CM 2

CRN 76-05-1

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RN 280553-83-5 CAPLUS

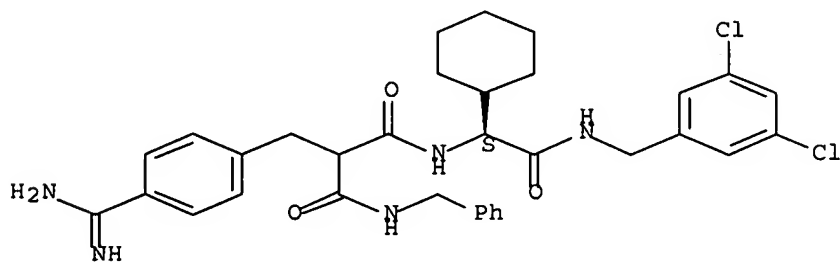
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CRN 280553-82-4

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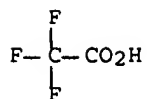
Absolute stereochemistry.



CM 2

CRN 76-05-1

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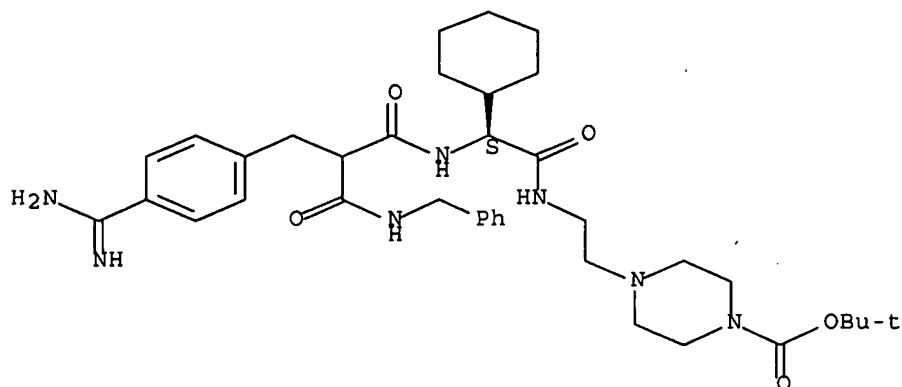
CN 1-Piperazinecarboxylic acid, 4-[2-[[[(2S)-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]cyclohexylacetyl]amino]ethyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 280553-84-6

CMF C37 H53 N7 O5

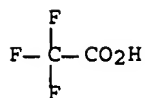
Absolute stereochemistry.



CM 2

CRN 76-05-1

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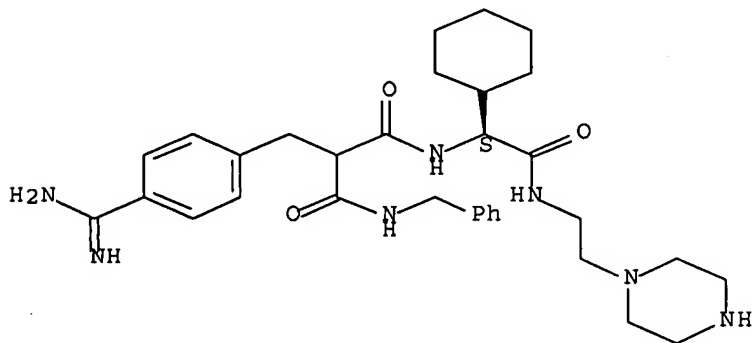
RN 280553-87-9 CAPLUS
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CM 1

CRN 280553-86-8

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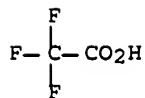
Absolute stereochemistry.



CM 2

CRN 76-05-1

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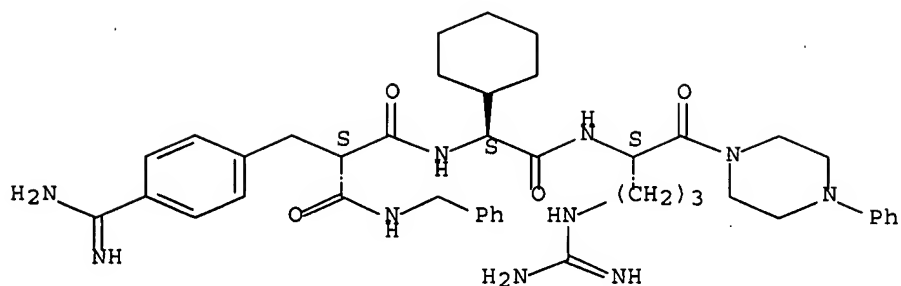
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CRN 280553-90-4

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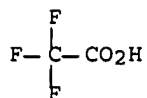
Absolute stereochemistry.



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CRN 76-05-1

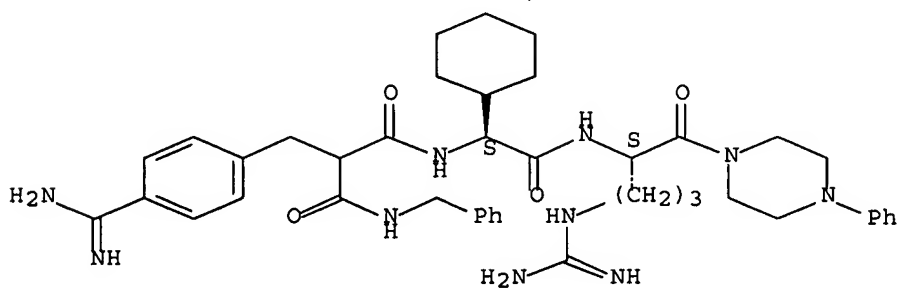
CMF C2 H F3 O2



RN 280553-96-0 CAPLUS

CN Glycinamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-
β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-
piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)- (9CI) (CA INDEX NAME)

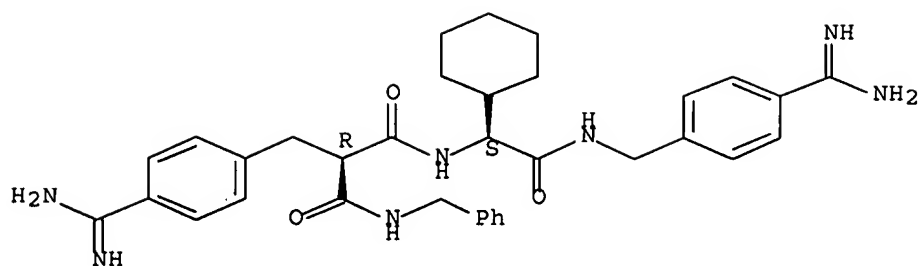
Absolute stereochemistry.



RN 280554-05-4 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-
(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-
(phenylmethyl)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 280554-33-8 CAPLUS

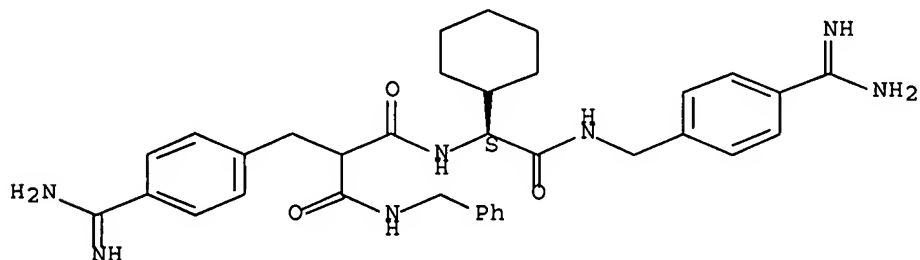
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280554-32-7

CMF C34 H41 N7 O3

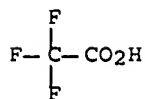
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 280554-35-0 CAPLUS

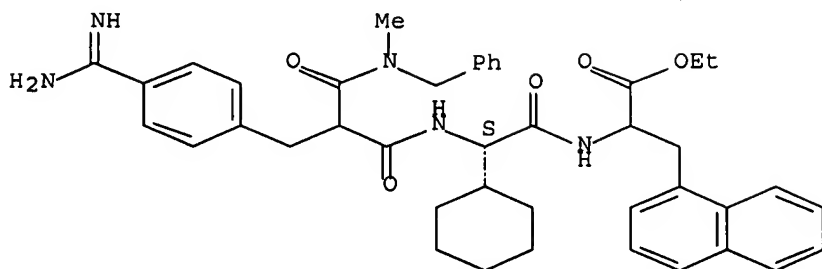
CN Alanine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM . 1

CRN 280554-34-9

CMF C42 H49 N5 O5

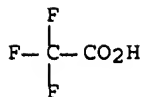
Absolute stereochemistry.



CM 2

CRN 76-05-1

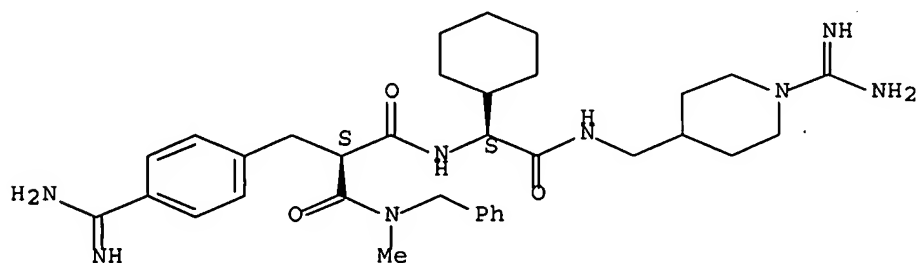
CMF C2 H F3 O2



RN 280554-36-1 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-methyl-N-(phenylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 280554-37-2 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-

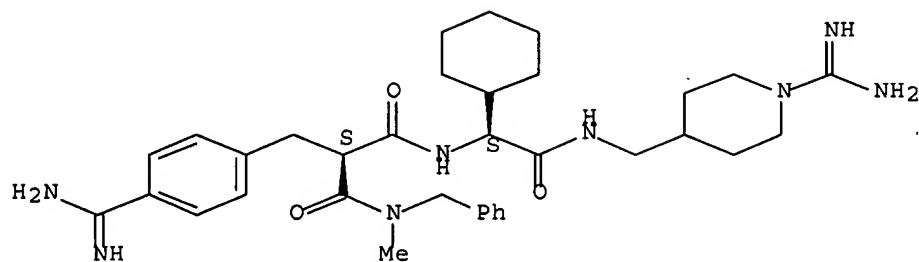
methyl-N-(phenylmethyl)-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280554-36-1

CMF C34 H48 N8 O3

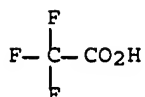
Absolute stereochemistry.



CM 2

CRN 76-05-1

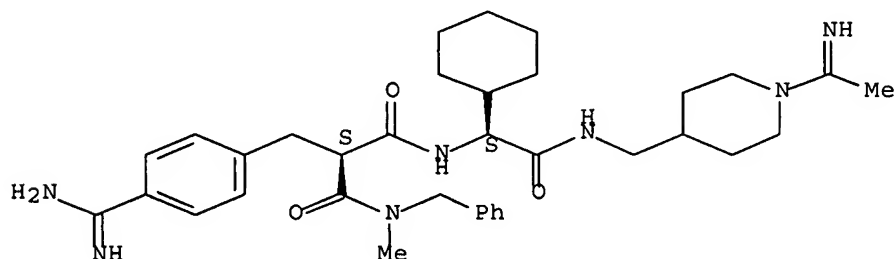
CMF C2 H F3 O2



RN 923294-55-7 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminoethyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2S)- (CA INDEX NAME)

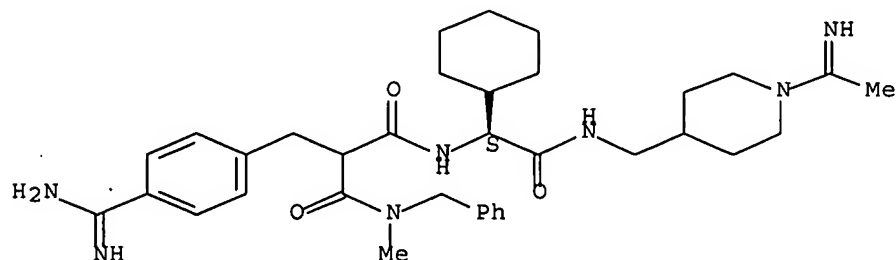
Absolute stereochemistry.



RN 923294-56-8 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminoethyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)- (CA INDEX NAME)

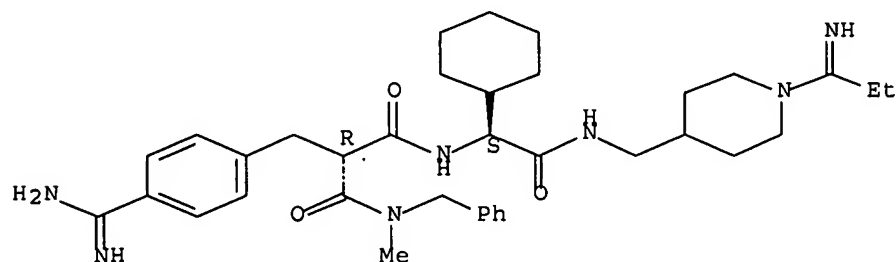
Absolute stereochemistry.



RN 923294-57-9 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminopropyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2R)- (CA INDEX NAME)

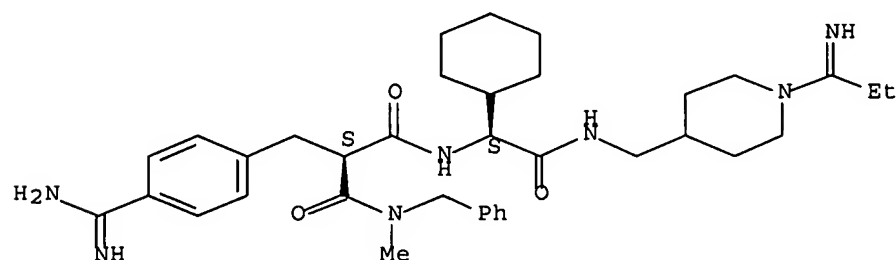
Absolute stereochemistry.



RN 923294-58-0 CAPLUS

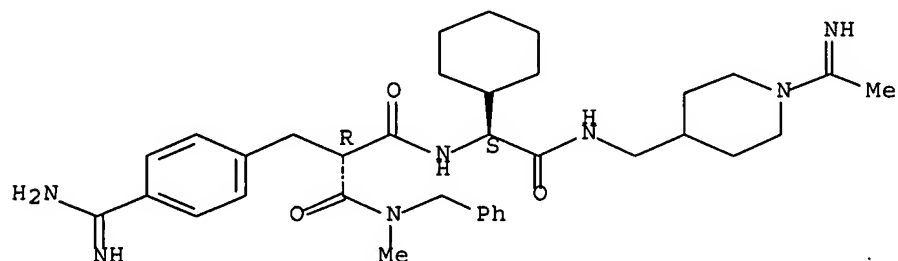
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminopropyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



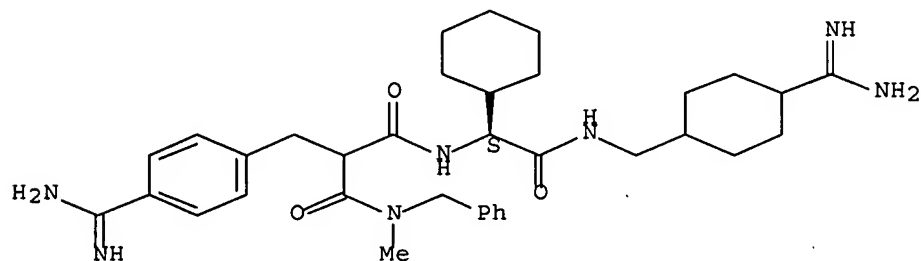
RN 923294-59-1 CAPLUS
 CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-[[[1-(1-iminoethyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-N1-methyl-N1-(phenylmethyl)-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 923586-00-9 CAPLUS
 CN Propanediamide, N3-[(1S)-2-[[[4-(aminoiminomethyl)cyclohexyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-2-[[4-(aminoiminomethyl)phenyl]methyl]-N1-methyl-N1-(phenylmethyl)- (CA INDEX NAME)

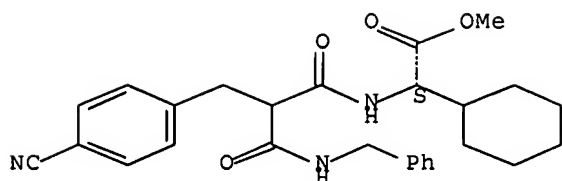
Absolute stereochemistry.



IT 280554-59-8P 280554-60-1P 280554-61-2P
 356545-90-9P 923294-54-6P 923585-99-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of malonic acid derivs. as factor Xa inhibitors and anticoagulant agents)

RN 280554-59-8 CAPLUS
 CN Cyclohexaneacetic acid, α -[[2-[[4-(cyanophenyl)methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

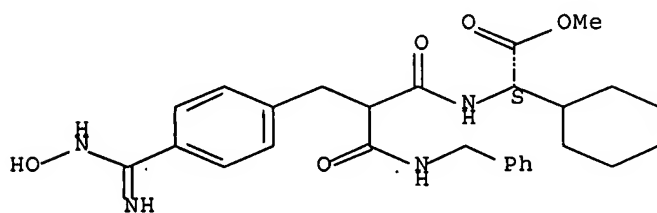
Absolute stereochemistry.



RN 280554-60-1 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

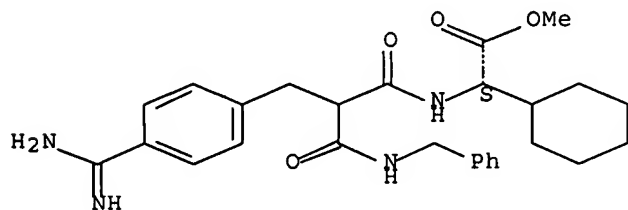
Absolute stereochemistry.



RN 280554-61-2 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

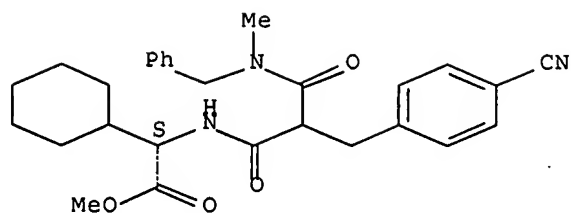
Absolute stereochemistry.



RN 356545-90-9 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-(4-cyanophenyl)methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 923294-54-6 CAPLUS

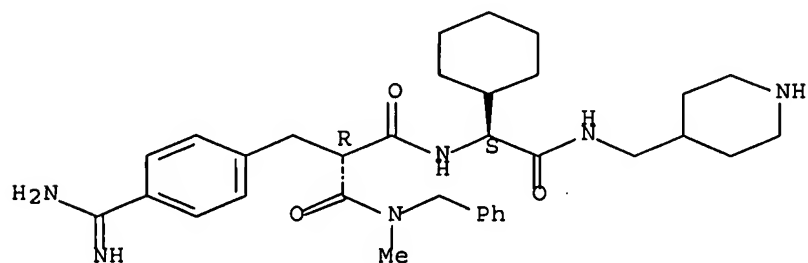
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-oxo-2-[(4-piperidinylmethyl)amino]ethyl]-N1-methyl-N1-(phenylmethyl)-, (2R)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 923294-53-5

CMF C33 H46 N6 O3

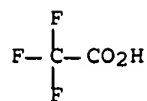
Absolute stereochemistry.



CM 2

CRN 76-05-1

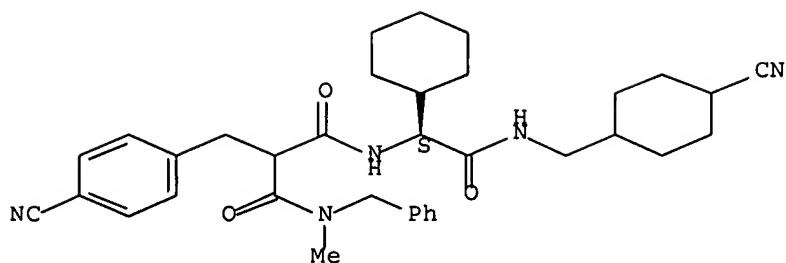
CMF C2 H F3 O2



RN 923585-99-3 CAPLUS

CN Propanediamide, N3-[(1S)-2-[[[(4-cyanocyclohexyl)methyl]amino]-1-cyclohexyl-2-oxoethyl]-2-[(4-cyanophenyl)methyl]-N1-methyl-N1-(phenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.



IT 923294-52-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of malonic acid derivs. as factor Xa inhibitors and
anticoagulant agents)

RN 923294-52-4 CAPLUS

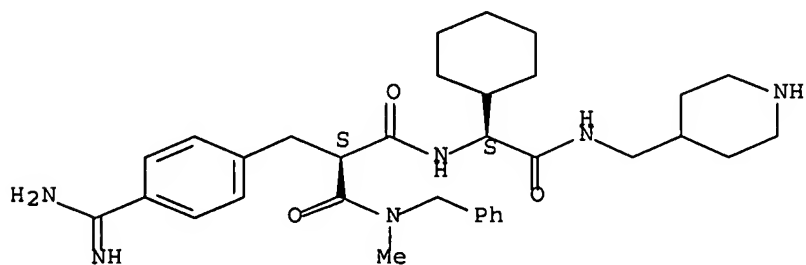
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N3-[(1S)-1-cyclohexyl-2-oxo-2-[(4-piperidinylmethyl)amino]ethyl]-N1-methyl-N1-(phenylmethyl)-, (2S)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 923294-51-3

CMF C33 H46 N6 O3

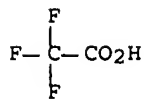
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



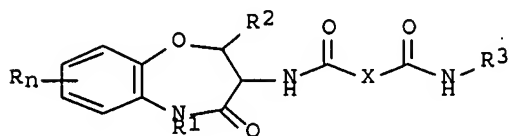
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS

L53 ANSWER 2 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2006:544815 CAPLUS Full-text
 DOCUMENT NUMBER: 145:28029
 TITLE: Preparation of oxaazabenzocycloheptyl malonamides as
 γ -secretase inhibitors.
 INVENTOR(S): Flohr, Alexander; Jakob-Roetne, Roland; Wostl,
 Wolfgang
 PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 58 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006122168	A1	20060608	US 2005-289176	20051130
US 7211573	B2	20070501		
WO 2006061136	A2	20060615	WO 2005-EP12834	20051201
WO 2006061136	A3	20060803		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
 KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
 MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
 SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
 VN, YU, ZA, ZM, ZW
 RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: EP 2004-106395 A 20041208
 EP 2005-100816 A 20050207
 OTHER SOURCE(S): MARPAT 145:28029
 GI



I

AB Title compds. [I; R = halo, (halo)alkyl; R1 = R, hydroxylalkyl, alkenyl, (halo)benzyl, cycloalkyl(alkyl), etc.; R2 = H, (halo- or hydroxy-substituted) alkyl, benzyl, cycloalkyl; R3 = (halo)alkyl, (halo)benzyl, cycloalkyl(alkyl), pyridyl(alkyl); X = CR4R4', CR4R4'O; R4, R4' = H, halo, alkyl, alkoxy, OH, etc.; n = 0-2], were prepared Thus, N-[(6R,7S)-2-fluoro-9-(2-hydroxyethyl)-6-methyl-8-oxo-6,7,8,9-tetrahydro-5-oxa-9-azabenzocyclohepten-7-yl]-2-(R or S)-

hydroxy-2-methyl-N-(2,2,3,3,3-pentafluoropropyl)malonamide entity A
(multistep preparation given) inhibited γ -secretase with $IC_{50} = 7$ nM.

IT 889457-84-5P 889457-85-6P

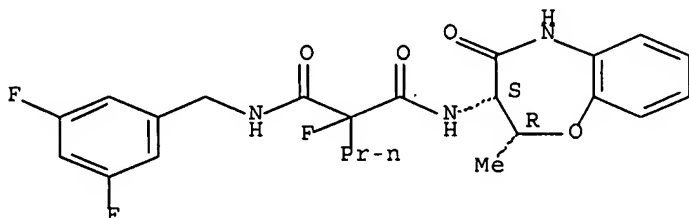
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(claimed compound; preparation of oxaazabenzocycloheptyl malonamides as
 γ -secretase inhibitors)

RN 889457-84-5 CAPLUS

CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-fluoro-2-propyl-N'-
[(2R,3S)-2,3,4,5-tetrahydro-2-methyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI)
(CA INDEX NAME)

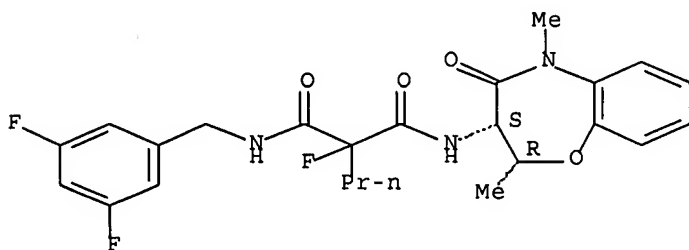
Absolute stereochemistry.



RN 889457-85-6 CAPLUS

CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-fluoro-2-propyl-N'-
[(2R,3S)-2,3,4,5-tetrahydro-2,5-dimethyl-4-oxo-1,5-benzoxazepin-3-yl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 889458-03-1P 889458-05-3P 889458-14-4P

889458-15-5P 889458-42-8P

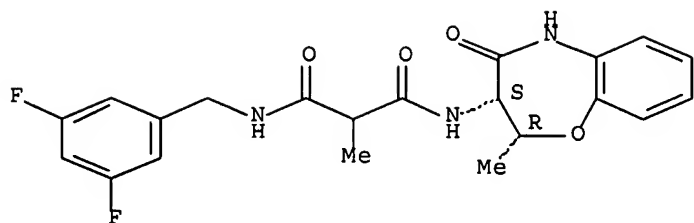
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of oxaazabenzocycloheptyl malonamides as γ -secretase
inhibitors)

RN 889458-03-1 CAPLUS

CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-methyl-N'-[(2R,3S)-
2,3,4,5-tetrahydro-2-methyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX
NAME)

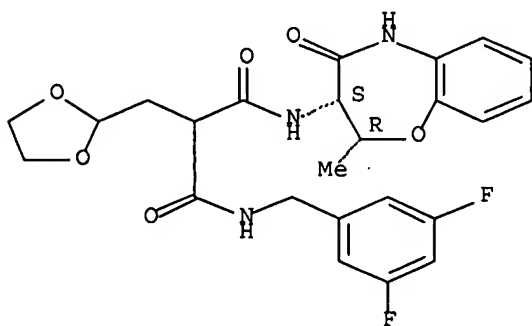
Absolute stereochemistry.



RN 889458-05-3 CAPLUS

CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-(1,3-dioxolan-2-ylmethyl)-N'-[(2R,3S)-2,3,4,5-tetrahydro-2-methyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

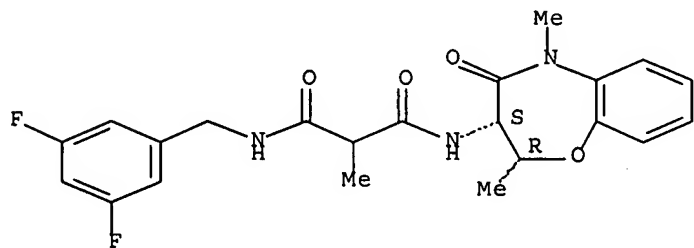
Absolute stereochemistry.



RN 889458-14-4 CAPLUS

CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-methyl-N'-[(2R,3S)-2,3,4,5-tetrahydro-2,5-dimethyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

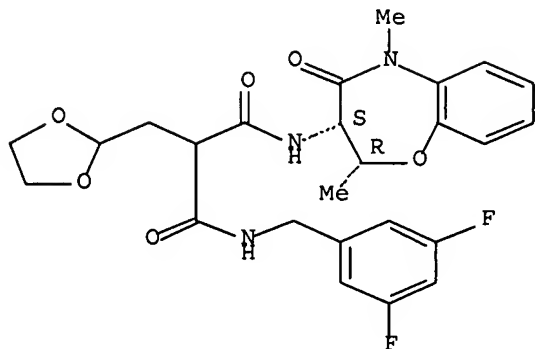
Absolute stereochemistry.



RN 889458-15-5 CAPLUS

CN Propanediamide, N-[(3,5-difluorophenyl)methyl]-2-(1,3-dioxolan-2-ylmethyl)-N'-[(2R,3S)-2,3,4,5-tetrahydro-2,5-dimethyl-4-oxo-1,5-benzoxazepin-3-yl]- (9CI) (CA INDEX NAME)

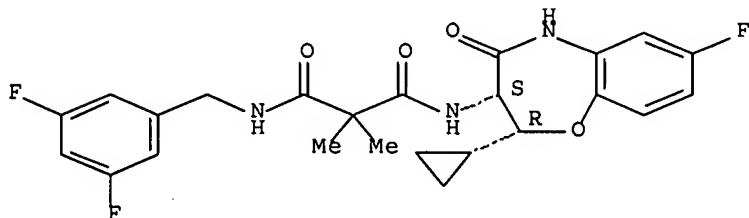
Absolute stereochemistry.



RN 889458-42-8 CAPLUS

CN Propanediamide, N-[(2R,3S)-2-cyclopropyl-7-fluoro-2,3,4,5-tetrahydro-4-oxo-1,5-benzoxazepin-3-yl]-N'-[(3,5-difluorophenyl)methyl]-2,2-dimethyl-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.



L53 ANSWER 3 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1314177 CAPLUS Full-text

DOCUMENT NUMBER: 144:51616

TITLE: Preparation of diazepinediones as ligands of melanocortin 1 and/or 4 receptors

INVENTOR(S): Szewczyk, Jerzy Ryszard; Speake, Jason Daniel; Sammond, Douglas Mccord; Sherrill, Ronald George

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005118573	A1	20051215	WO 2005-US18773	20050527
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,				

SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
 ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
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PRIORITY APPLN. INFO.:

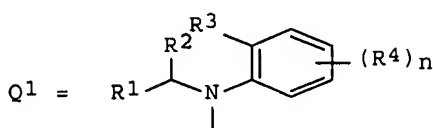
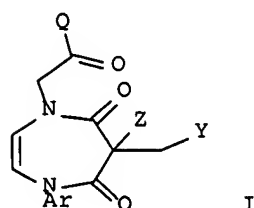
US 2004-575644P

P 20040528

OTHER SOURCE(S):

MARPAT 144:51616

GI



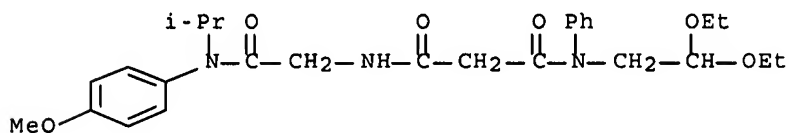
AB Title compds. [I; Ar = (substituted) aryl, heteroaryl; Y = specified indazolyl, benzimidazolyl, oxobenzimidazolyl; Z = H, alkoxy; Q = Q1; R1, R2, R4 = H, OH, haloalkyl, alkoxy, haloalkoxy, amino; n = 0-2; R3 = H; R2R3 = atoms to form 6-7 membered ring], were prepared Thus, 2-[2,4-dioxo-3-(1H-indazol-3-ylmethylene)-5-phenyl-2,3,4,5-tetrahydro-1H-1,5-diazepin-1-yl]-N-(4-chlorophenyl)-N-isopropylacetamide hydrochloride (multistep preparation given) showed MC4R agonist activity with pEC50 = 7.37.

IT 179083-73-9P 179083-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of diazepinediones as ligands of melanocortin-1 and/or 4 receptors)

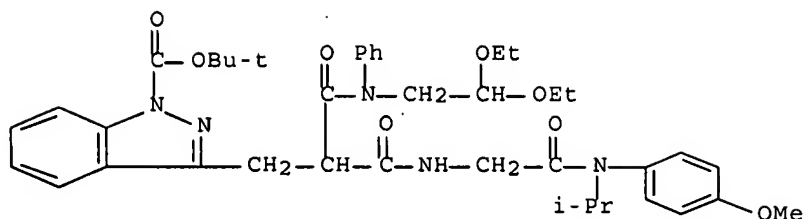
RN 179083-73-9 CAPLUS

CN Glycinamide, N-(2,2-diethoxyethyl)-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 179083-74-0 CAPLUS

CN Glycinamide, N-(2,2-diethoxyethyl)-2-[[1-[(1,1-dimethylethoxy)carbonyl]-1H-indazol-3-yl]methyl]-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



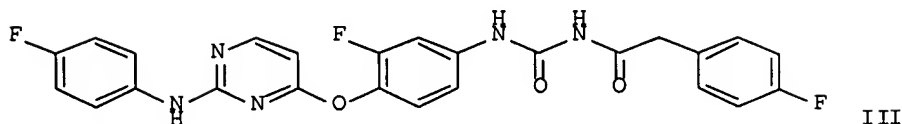
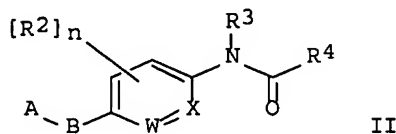
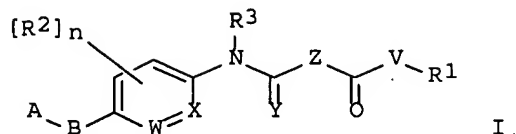
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L53 ANSWER 4 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:1176889 CAPLUS Full-text
 DOCUMENT NUMBER: 143:440434
 TITLE: Preparation of monocyclic heterocycles as kinase inhibitors, particularly Met kinase, for treating cancer
 INVENTOR(S): Borzilleri, Robert M.; Cornelius, Lyndon A. M.; Schmidt, Robert J.; Schroeder, Gretchen M.; Kim, Kyoung S.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 128 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005245530	A1	20051103	US 2005-111144	20050421
AU 2005249382	A1	20051215	AU 2005-249382	20050422
CA 2563831	A1	20051215	CA 2005-2563831	20050422
WO 2005117867	A2	20051215	WO 2005-US14120	20050422
WO 2005117867	A3	20060330		
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1737451	A2	20070103	EP 2005-779444	20050422
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NO 2006005148	A	20061108	NO 2006-5148	20061108
PRIORITY APPLN. INFO.:				
			US 2004-564842P	P 20040423
			US 2004-639178P	P 20041223
			US 2005-111144	A 20050421
			WO 2005-US14120	W 20050422

OTHER SOURCE(S):
GI

MARPAT 143:440434



AB The invention is related to compds. of formula I and II [wherein R1 = H, (un)substituted alk(en/yn)yl, hetero/aryl, etc.; each R2 = independently H, halo, CN, NO2, alkyl, etc.; B = O, S, SO, SO2, NH, etc.; V = NH and derivs., (CH2)p and derivs. with proviso; p = 0-4; W, X = independently C, N; Z = CH2 and derivs.; (CH2)q-NH and derivs.; q = 0-2; R3 = H, (un)substituted heterocyclyl, alk(en/yn)yl, cycloalkyl, hetero/aryl, etc.; R4 = (un)substituted hetero/aryl, heterocycloalkyl with provisos; A = (un)substituted pyridin-4-yl, pyrimidin-4-yl, pyridazin-4-yl, etc.] their enantiomers, diastereomers, hydrates, solvates, and pharmaceutically acceptable salts, as protein kinase, particularly Met kinase, inhibitors and methods for using them for the treatment of cancer. E.g., a 4 step synthesis of pyrimidine II, starting from 2,4-dichloropyrimidine and N-(3-fluoro-4-hydroxyphenyl)acetamide, was given. Preferred compds. I inhibited Met kinase with IC50 values between 0.01 and 100 μ M.

IT 868736-02-1P

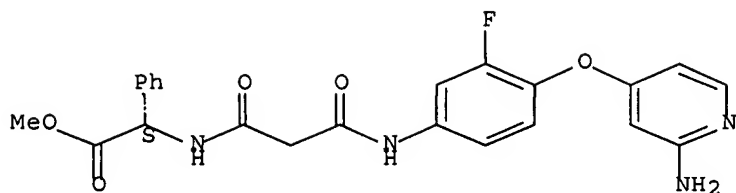
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of monocyclic heterocycles as kinase inhibitors
for treating cancer)

RN 868736-02-1 CAPLUS

CN Benzeneacetic acid, α -[[3-[[4-[(2-amino-4-pyridinyl)oxy]-3-fluorophenyl]amino]-1,3-dioxopropyl]amino]-, methyl ester, monohydrochloride, (α S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

IT 868736-03-2P

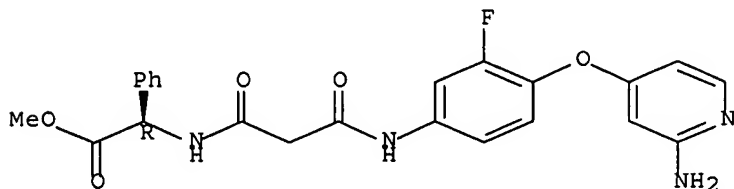
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of monocyclic heterocycles as kinase inhibitors for treating cancer)

RN 868736-03-2 CAPLUS

CN Benzeneacetic acid, α -[[3-[[4-[(2-amino-4-pyridinyl)oxy]-3-fluorophenyl]amino]-1,3-dioxopropyl]amino]-, methyl ester, monohydrochloride, (α R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L53 ANSWER 5 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:323777 CAPLUS Full-text

DOCUMENT NUMBER: 142:378922

TITLE: Method for decreasing sebum production using malonamide acyl CoA cholesterol acyl transferase inhibitors

INVENTOR(S): Kostlan, Catherine R.; Raheja, Raj Neil; Tugnait, Meera; Wade, Kimberly

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 17 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2005079144	A1	20050414	US 2004-958306	20041005
AU 2004280134	A1	20050421	AU 2004-280134	20040927
CA 2541814	A1	20050421	CA 2004-2541814	20040927
WO 2005034931	A1	20050421	WO 2004-IB3156	20040927

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1673077	A1	20060628	EP 2004-769499	20040927
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

CN 1863521	A	20061115	CN 2004-80029467	20040927
BR 2004015136	A	20061128	BR 2004-15136	20040927
JP 2007508291	T	20070405	JP 2006-530738	20040927
NO 2006001277	A	20060629	NO 2006-1277	20060321

PRIORITY APPLN. INFO.: US 2003-509984P P 20031009
WO 2004-IB3156 W 20040927

OTHER SOURCE(S): MARPAT 142:378922

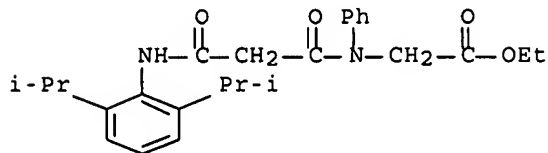
AB The present invention is directed to the topical application of the malonamide acyl CoA cholesterol acyl transferase (ACAT) inhibitors. Other aspects of the invention are directed to topical formulations of these diamides, their use to treat sebaceous gland disorders and their use to alleviate oily skin. Efficacy of a series of ACAT inhibitors in decreasing sebum production in hamster ear sebaceous glands is shown.

IT 137379-32-9

RL: COS (Cosmetic use); PAC (Pharmacological activity); BIOL (Biological study); USES (Uses)
(method for decreasing sebum production using malonamide acyl CoA cholesterol acyl transferase inhibitors)

RN 137379-32-9 CAPLUS

CN Glycine, N-[3-[[2,6-bis(1-methylethyl)phenyl]amino]-1,3-dioxopropyl]-N-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 6 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:652532 CAPLUS Full-text

DOCUMENT NUMBER: 141:172870

TITLE: Conjugates of haptens and β -lactam derivatives for quantifying haptens in solution and device for implementation thereof

INVENTOR(S): Kohl, Michel; Renotte, Roger; Sarlet, Guy; Lejeune,

PATENT ASSIGNEE(S): Robert; Granier, Benoit
 SOURCE: Belg.
 U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S.
 Ser. No. 171,819.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004157262	A1	20040812	US 2001-915211	20010725
BE 1010184	A3	19980203	BE 1996-384	19960430
US 6436649	B1	20020820	US 1999-171819	19990611
PRIORITY APPLN. INFO.:			BE 1996-384	A 19960430
			US 1999-171819	A2 19990611
			WO 1997-BE52	W 19970430

AB The present invention is related to a conjugate of a hapten to a natural or synthetic β -lactam derivative, comprising at least a side chain, wherein the side chain of the β -lactam derivative is at least partially constitutive of the conjugating arm. The invention relates also to a method for the immunoassay of the hapten involving said β -lactam derivative-hapten conjugate as an inhibitor for a lactamase or a penicillin detector capable of specific recognition of the β -lactamic moiety of said conjugate. The hapten is a steroid, drug of abuse and medicine e.g. nandrolone, testosterone, progesterone, estradiol and cocaine; and the β -lactam derivative is a penicillin derivative or cephalosporin derivative e.g. carbenicillin, oxacillin, cefuroxime, cefotaxime, methicillin, benzylpenicillin and phenoxymethylpenicillin.

IT 198830-23-8P

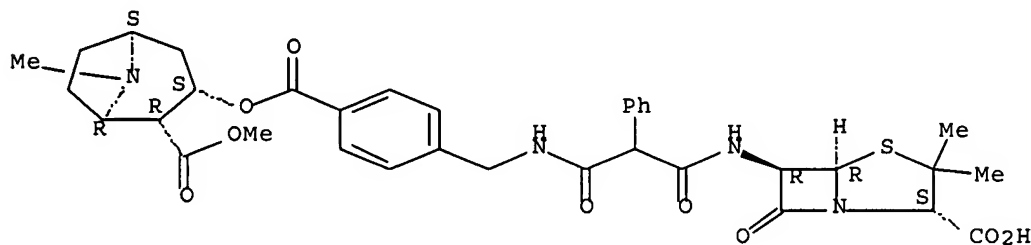
RL: ARU (Analytical role, unclassified); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(conjugates of haptens and β -lactam derivs. for quantifying haptens in solution and device for implementation thereof)

RN 198830-23-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[[4-[[[3-[[[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]amino]-1,3-dioxo-2-phenylpropyl]amino]methyl]benzoyl]oxy]-8-methyl-, 2-methyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 2004:648538 CAPLUS Full-text

DOCUMENT NUMBER: 141:191072

TITLE: Preparation and use of chemically-modified metabolites of regulatory peptides

INVENTOR(S): Peri, Krishna; Habi, Abdelkrim; Gravel, Denis

PATENT ASSIGNEE(S): Theratechnologies Inc., Can.

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004067548	A2	20040812	WO 2004-CA131	20040130
WO 2004067548	A3	20041209		
WO 2004067548	B1	20050217		

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US 2005059605	A1	20050317	US 2004-768974	20040130
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PRIORITY APPLN. INFO.: US 2003-443860P P 20030131

OTHER SOURCE(S): MARPAT 141:191072

AB The invention relates to peptides B-A-CO-P or their pharmaceutically-acceptable salts, where P is a dipeptidyl-peptidase (DPPIV) peptide metabolite of regulatory peptides obtained by cleavage of the two N-terminal amino acids, A is (hetero)alk(en)(yn)ylene or Ph and B is (un)substituted (hetero)aryl or cycloalkyl. More specifically, the invention relates to conferring biol. activity to metabolites of regulatory peptides by the covalent coupling of small mols. Thus, 3-(4-methoxyphenethylamino)-3-oxopropanoyl-GLP-1 (9-36) was prepared by solid-phase peptide chemical and N-acylation and shown to produce a more significant hypoglycemic response in mice compared to native GLP-1.

IT 736176-31-1P 736176-32-2P 736176-38-8P

736176-39-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

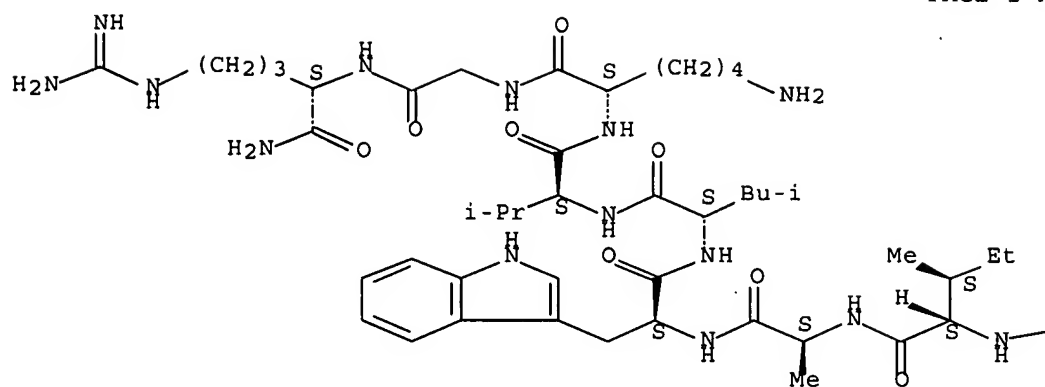
(preparation and use of chemical-modified metabolites of regulatory peptides)

RN 736176-31-1 CAPLUS

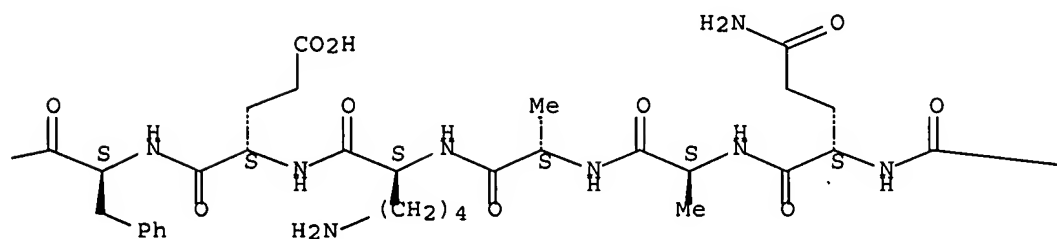
CN L-Argininamide, 3-oxo-N-(2-phenylethyl)- β -alanyl-L- α -glutamylglycyl-L-threonyl-L-phenylalanyl-L-threonyl-L-seryl-L- α -aspartyl-L-valyl-L-seryl-L-seryl-L-tyrosyl-L-leucyl-L- α -glutamylglycyl-L-glutaminyl-L-alanyl-L-alanyl-L-lysyl-L- α -glutamyl-L-phenylalanyl-L-isoleucyl-L-alanyl-L-tryptophyl-L-leucyl-L-valyl-L-lysylglycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

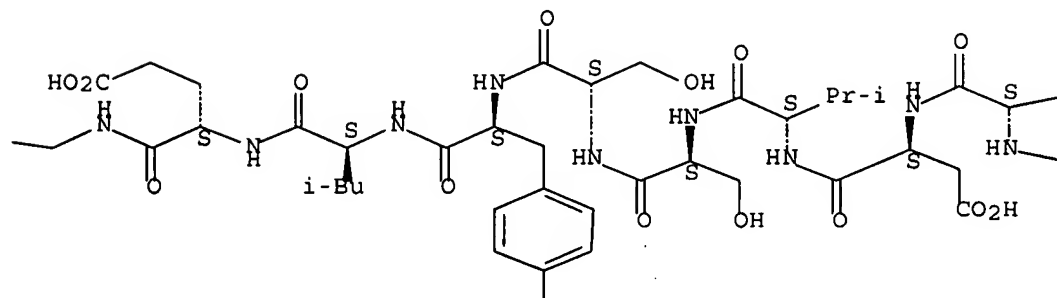
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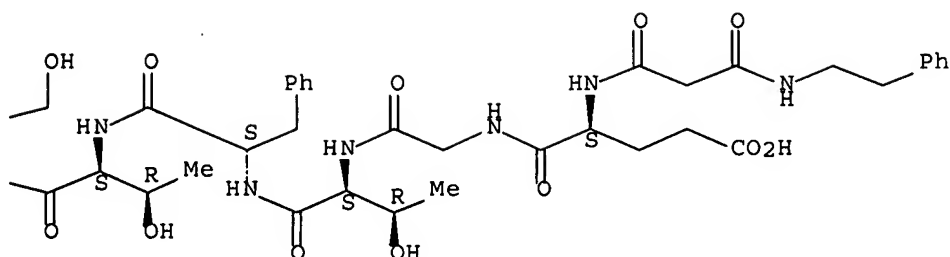
PAGE 1-B



PAGE 1-C



PAGE 1-D



PAGE 2-C

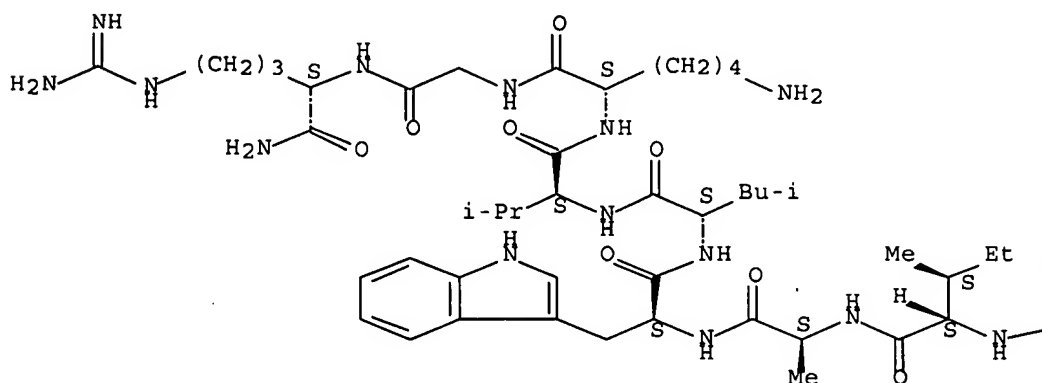


RN 736176-32-2 CAPLUS

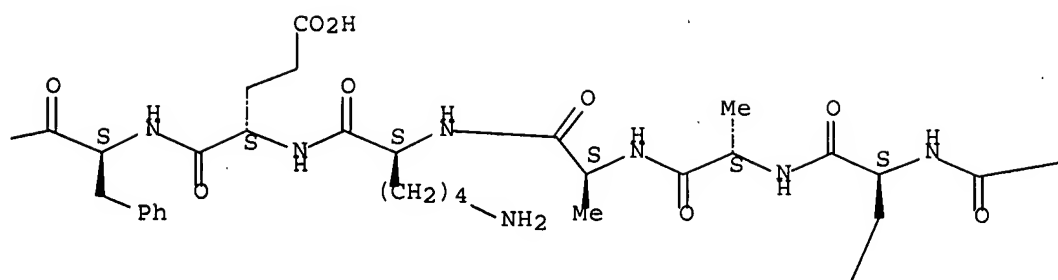
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Absolute stereochemistry.

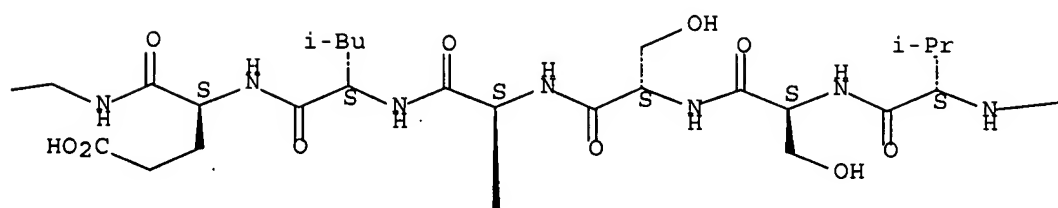
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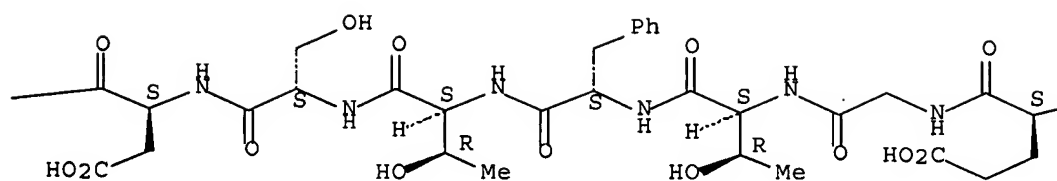
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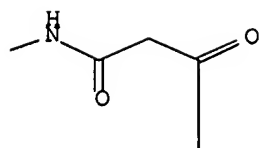
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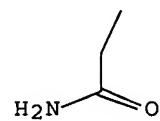
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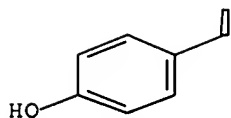
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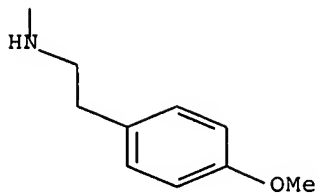
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PAGE 2-C



PAGE 2-E

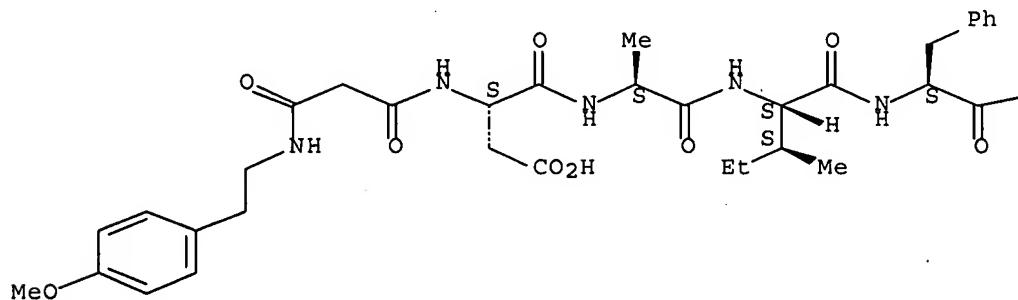


RN 736176-38-8 CAPLUS

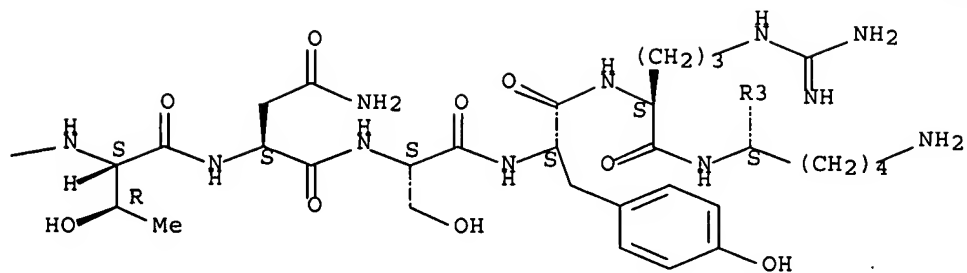
CN L-Argininamide, N-[2-(4-methoxyphenyl)ethyl]-3-oxo- β -alanyl-L- α -aspartyl-L-alanyl-L-isoleucyl-L-phenylalanyl-L-threonyl-L-asparaginyll-L-seryl-L-tyrosyl-L-arginyl-L-lysyl-L-valyl-L-leucylglycyl-L-glutaminyll-L-leucyl-L-seryl-L-alanyl-L-arginyl-L-lysyl-L-leucyl-L-leucyl-L-glutaminyll-L- α -aspartyl-L-isoleucyl-L-methionyl-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

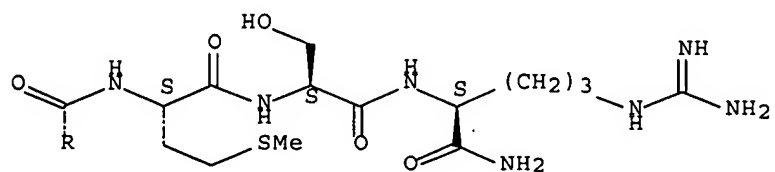
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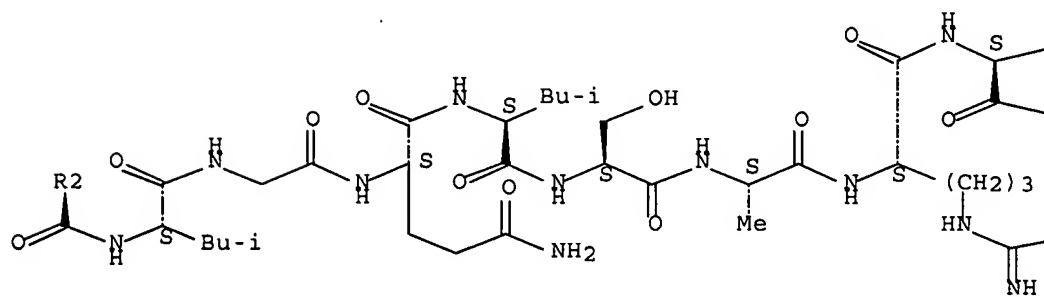
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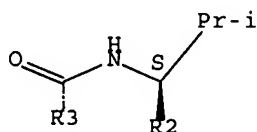
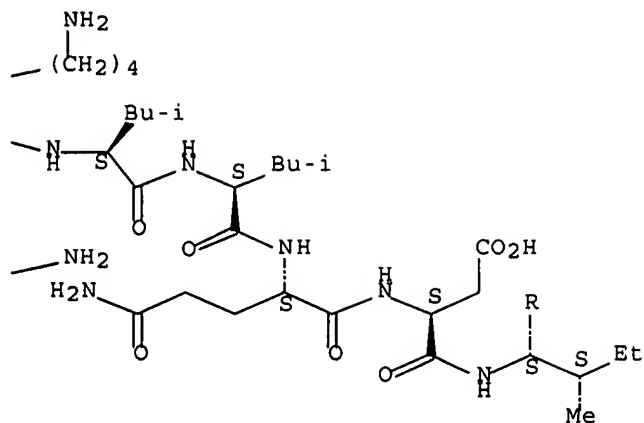


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PAGE 3-A

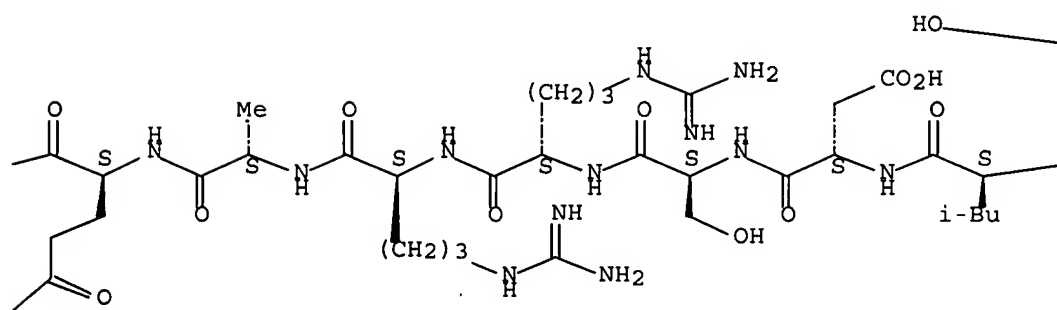
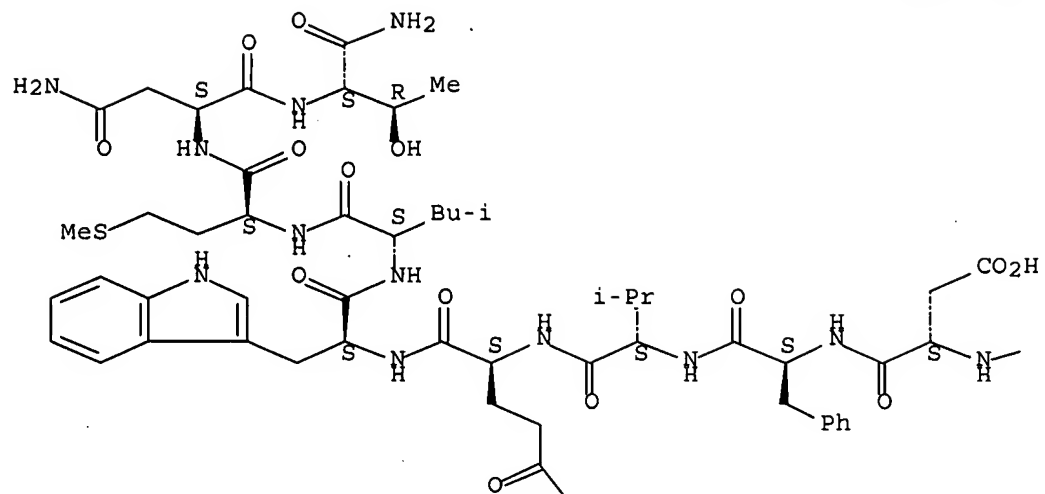




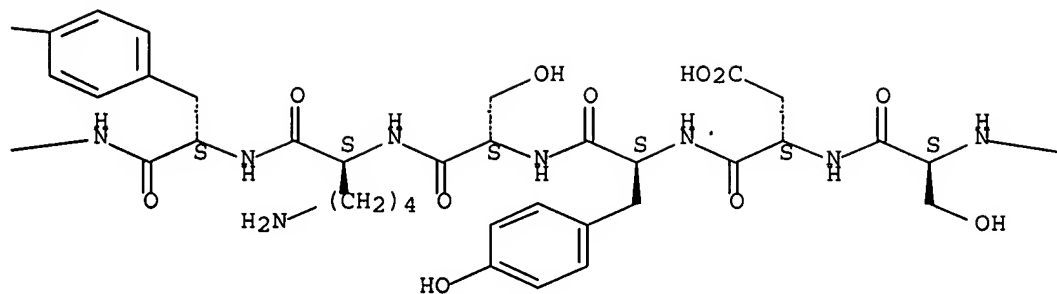
RN 736176-39-9 CAPLUS

CN L-Threoninamide, N-[2-(4-methoxyphenyl)ethyl]-3-oxo-β-alanyl-L-glutaminylglycyl-L-threonyl-L-phenylalanyl-L-threonyl-L-seryl-L-α-aspartyl-L-tyrosyl-L-seryl-L-lysyl-L-tyrosyl-L-leucyl-L-α-aspartyl-L-seryl-L-arginyl-L-arginyl-L-alanyl-L-glutaminyl-L-α-aspartyl-L-phenylalanyl-L-valyl-L-glutaminyl-L-tryptophyl-L-leucyl-L-methionyl-L-asparaginyl- (9CI) (CA INDEX NAME)

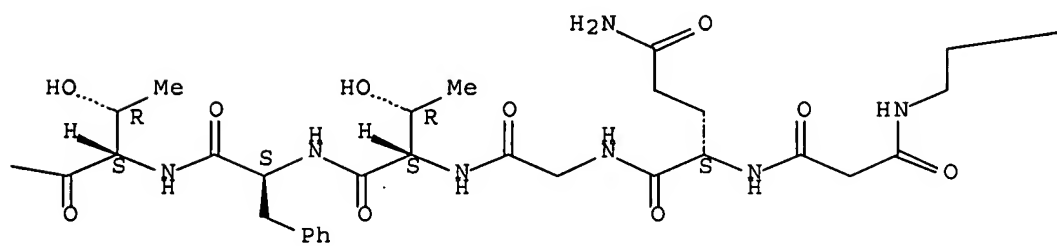
Absolute stereochemistry.



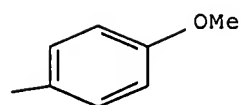
PAGE 1-C



PAGE 1-D



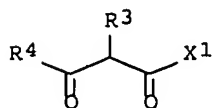
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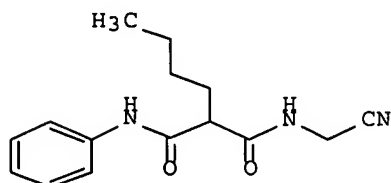
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L53 ANSWER 8 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:946095 CAPLUS Full-text
 DOCUMENT NUMBER: 138:24322
 TITLE: Preparation of malonamides as cathepsin inhibitors
 INVENTOR(S): Patterson, John W.; Zipfel, Sheila
 PATENT ASSIGNEE(S): Celera, USA
 SOURCE: PCT Int. Appl., 67 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002098406	A1	20021212	WO 2002-US17922	20020604
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2449021	A1	20021212	CA 2002-2449021	20020604
AU 2002312357	A1	20021216	AU 2002-312357	20020604
EP 1399146	A1	20040324	EP 2002-739721	20020604
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2002010172	A	20040622	BR 2002-10172	20020604
CN 1512880	A	20040714	CN 2002-811289	20020604
JP 2005500275	T	20050106	JP 2003-501445	20020604
NZ 529903	A	20050930	NZ 2002-529903	20020604
US 2004147503	A1	20040729	US 2003-478632	20031124
NO 2003005365	A	20040220	NO 2003-5365	20031202
ZA 2003009371	A	20050527	ZA 2003-9371	20031202
IN 2003DN02092	A	20060120	IN 2003-DN2092	20031204
PRIORITY APPLN. INFO.:			US 2001-295744P	P 20010604
			WO 2002-US17922	W 20020604
OTHER SOURCE(S):	MARPAT 138:24322			
GI				



I



II

AB The title malonamides I [wherein X1 = substituted amino; R3 = (un)substituted alkyl; R4 = (un)substituted amino; with provisos; and the N-oxide derivs., prodrugs, protected derivs., isomers, mixts. of isomers, pharmaceutically acceptable salts, and solvates thereof] were prepared as selective cathepsin S inhibitors. For example, a solution of aniline in CH₂Cl₂ was treated with Me malonyl chloride in the presence of Et₃N, followed by reaction with 1-iodobutane in N-methylpyrrolidinone in the presence of LiOH to give Me 2-phenylcarbamoylhexanoate. The above compound was treated with NaOH in MeOH, followed by the addition of 1 N aqueous HCl solution to afford 2-phenylcarbamoylhexanoic acid (74%). The hexanoic acid in DMF was treated with PyBOP, aminoacetonitrile bisulfate, and Et₃N to provide 2-butyl-N-cyanomethyl-N'-phenylmalonamide (II) (57%). I showed inhibition consts. against cathepsin S in the range of 10⁻¹⁰ M to 10⁻⁷ M. Pharmaceutical formulations containing a compound of formula I were also presented.

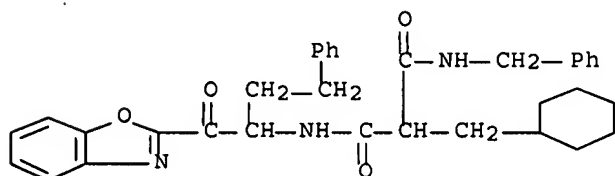
IT 477860-82-5P 477861-17-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cathepsin inhibitor; preparation of malonamides via condensation reactions of malonic acids with amines as cathepsin inhibitors)

RN 477860-82-5 CAPLUS

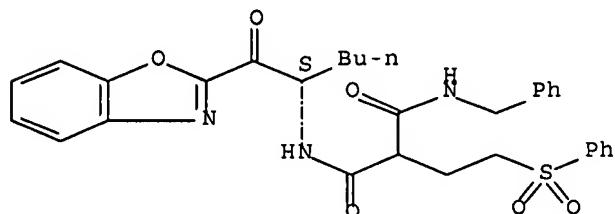
CN Propanediamide, N-[1-(2-benzoxazolylcarbonyl)-3-phenylpropyl]-2-(cyclohexylmethyl)-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 477861-17-9 CAPLUS

CN Propanediamide, N-[(1S)-1-(2-benzoxazolylcarbonyl)pentyl]-N'-(phenylmethyl)-2-[2-(phenylsulfonyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 9 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:631914 CAPLUS Full-text

DOCUMENT NUMBER: 135:195426

TITLE: Preparation of malonic acid amide derivatives as inhibitors of blood clotting factor Xa

INVENTOR(S): Al-Obeidi, Fahad; Walser, Armin; Wildgoose, Peter

PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany

SOURCE: Eur. Pat. Appl., 69 pp.

CODEN: EPXXDW

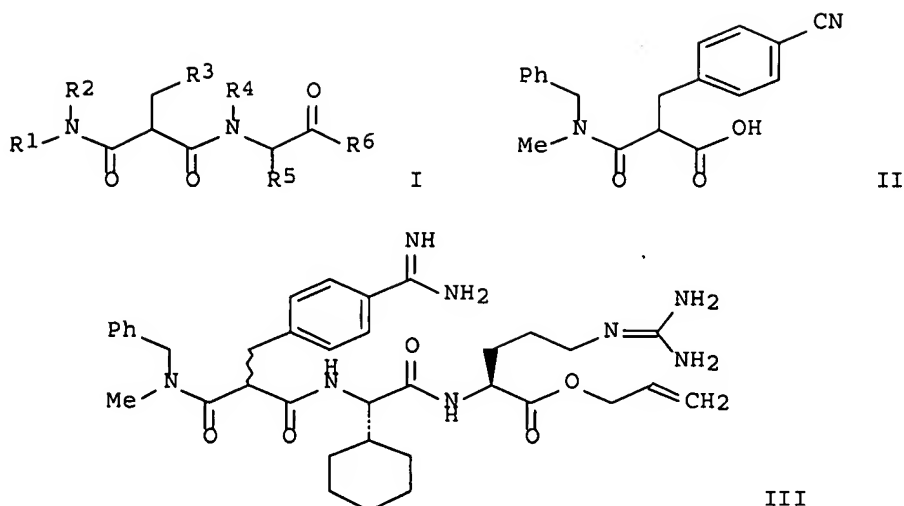
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1127884	A1	20010829	EP 2000-104041	20000226
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2001008694	A	20021210	BR 2001-8694	20010121
CA 2400871	A1	20010830	CA 2001-2400871	20010221
WO 2001062735	A1	20010830	WO 2001-EP1928	20010221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1265867	A1	20021218	EP 2001-907546	20010221
EP 1265867	B1	20051228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 200300080	A2	20030628	HU 2003-80	20010221
JP 2003524001	T	20030812	JP 2001-562517	20010221
NZ 520982	A	20040528	NZ 2001-520982	20010221
AT 314350	T	20060115	AT 2001-907546	20010221
ES 2254370	T3	20060616	ES 2001-1907546	20010221
US 2002022596	A1	20020221	US 2001-790641	20010223
US 6794365	B2	20040921		
ZA 2002006581	A	20030728	ZA 2002-6581	20020816
NO 2002004040	A	20020924	NO 2002-4040	20020823
PRIORITY APPLN. INFO.:			EP 2000-104041	A 20000226
			WO 2001-EP1928	W 20010221
OTHER SOURCE(S):			MARPAT 135:195426	
GI				



AB Title compds. I [R1 = H, alk(en)yl, aryl(alkyl); R2 = H, alkyl; R3 = aryl; R4 = H, alkyl, etc.; R5 = (cyclo)alkyl, cycloalkyl-alkyl, aryl(alkyl), etc.; R6 = NH₂, OH or substituted derivs.] are prepared. Examples included 3 synthetic procedures (including a general solid phase method), over 100 compds. prepared and 8 bioassays (data provided for 1 of the bioassays). For instance, benzyl Me amine was treated with bis(trimethylsilyl)acetamide (DCM, reflux, 3 h) followed by addition of 4-[(2,2-dimethyl-4,6-dioxo-1,3-dioxan-5-yl)methyl]benzonitrile (DCM, reflux, 3 h) to give II. II was coupled to (αS)-amino-cyclohexane- acetic acid Me ester (iPr₂EtN, HODhbt, DCC, DMF, 10°C) and the resulting amide-nitrile reacted with excess hydroxylamine (EtOH, reflux, 4 h) to give the corresponding N-hydroxy carbamimidoyl derivative. This intermediate was deoxygenated (Pd-H₂/C), hydrolyzed (HCl_{aq}, CH₃CN, 4 days @ room temperature) and coupled with (S)-2-amino-5-guanidinopentanoic acid allyl ester (DMF, collidine, HATU) to give III. Isomers of III were separated by chromatog. (MPLC, RP18) and isolated as the trifluoroacetic acid salts. An isomer of III had K_i = 0.0010 μM for factor Xa. The invention also provides methods for the treatment/prevention of (e.g.) thromboembolic diseases.

IT 356543-22-1P 356543-24-3P 356543-26-5P
 356543-28-7P 356543-36-7P 356543-38-9P
 356543-46-9P 356543-51-6P 356543-57-2P
 356543-69-6P 356543-75-4P 356543-83-4P
 356543-91-4P 356543-99-2P 356544-07-5P
 356544-15-5P 356544-24-6P 356544-32-6P
 356544-36-0P 356544-52-0P 356544-62-2P
 356544-68-8P 356544-74-6P 356544-80-4P
 356545-29-4P 356545-35-2P 356545-43-2P
 356545-45-4P 356545-47-6P 356545-53-4P
 356545-55-6P 356545-60-3P 356545-66-9P
 356545-67-0P 356545-69-2P 356545-71-6P
 356545-73-8P 356545-75-0P 356545-77-2P
 356545-79-4P 356545-81-8P 356545-83-0P
 356545-85-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug; preparation of malonic acid amide derivs. as inhibitors of blood clotting factor Xa)

RN 356543-22-1 CAPLUS

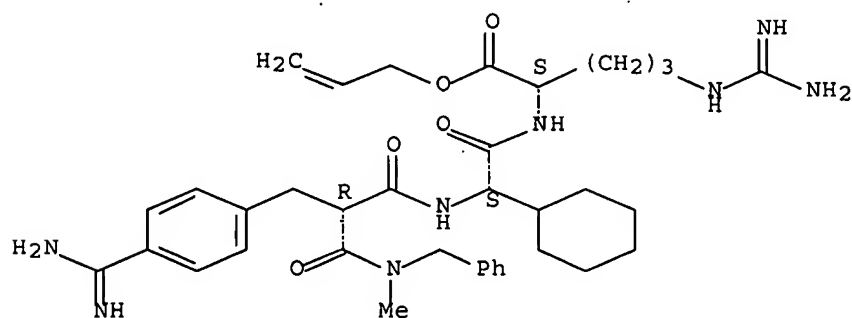
CN L-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, 2-propenyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

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CRN 356543-21-0

CMF C36 H50 N8 O5

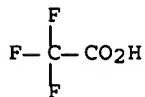
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356543-24-3 CAPLUS

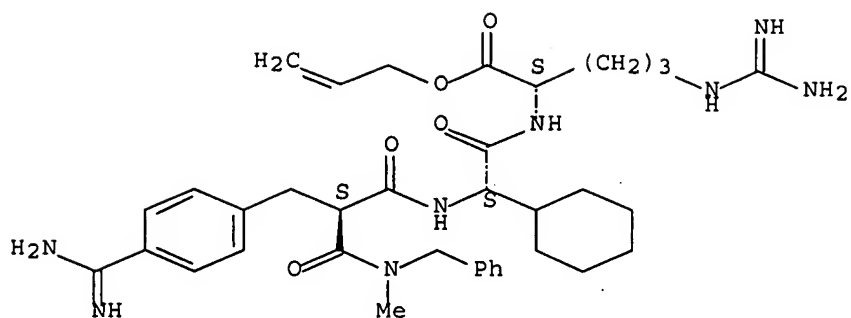
CN L-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, 2-propenyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356543-23-2

CMF C36 H50 N8 O5

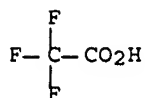
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356543-26-5 CAPLUS

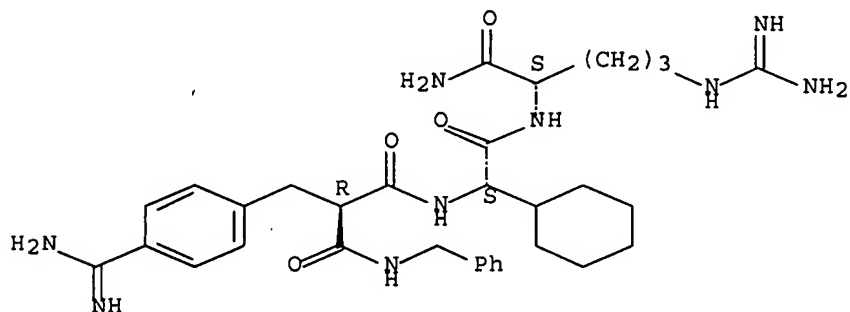
CN L-Argininamide, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356543-25-4

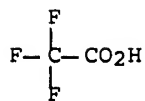
CMF C32 H45 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

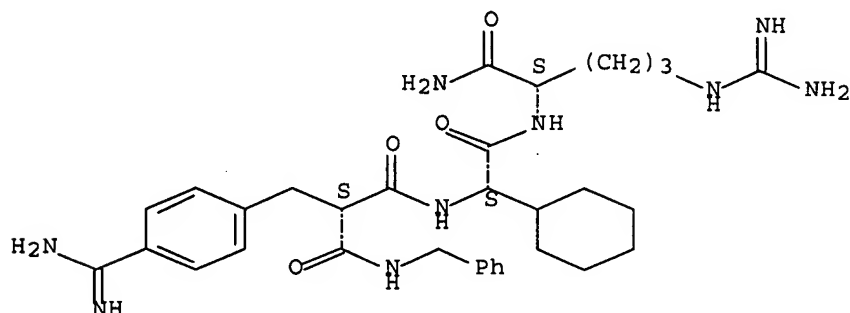


RN 356543-28-7 CAPLUS
CN L-Argininamide, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

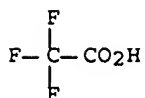
CRN 356543-27-6
CMF C32 H45 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

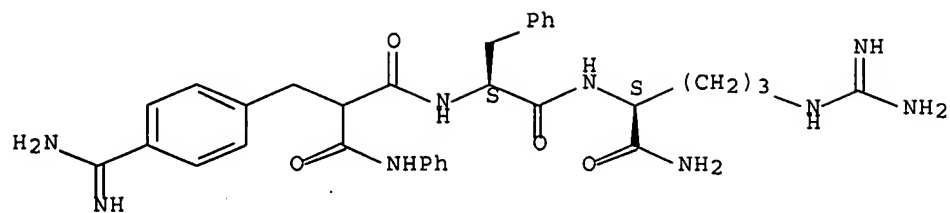


RN 356543-36-7 CAPLUS
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-L-phenylalanyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

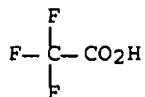
CRN 356543-35-6
CMF C32 H39 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

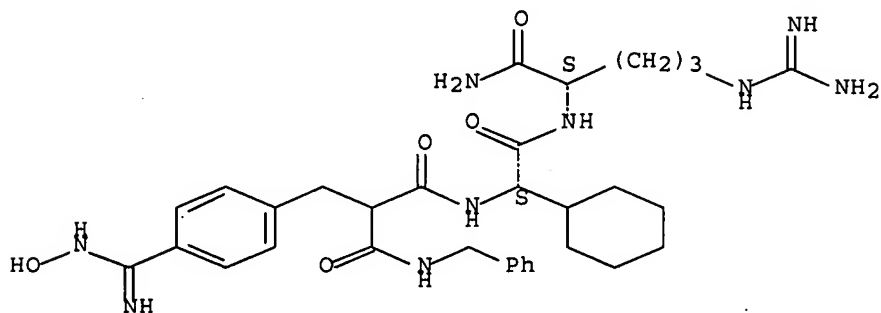


RN 356543-38-9 CAPLUS
CN L-Argininamide, 2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-oxo-N-(phenylmethyl)- β -alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 356543-37-8
CMF C32 H45 N9 O5

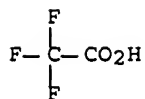
Absolute stereochemistry.



CM 2

CRN 76-05-1

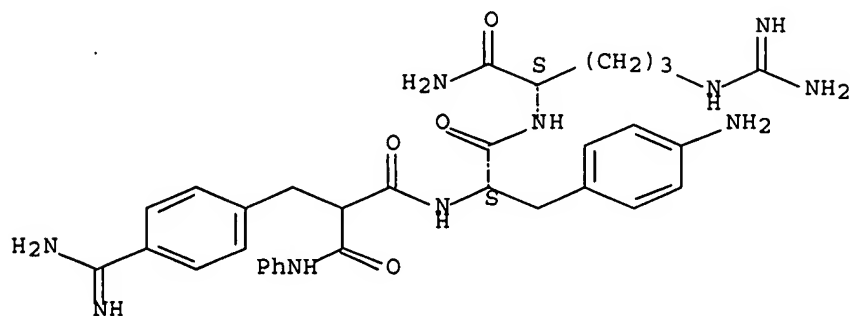
CMF C2 H F3 O2



RN 356543-46-9 CAPLUS

CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
β-alanyl-4-amino-L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 356543-51-6 CAPLUS

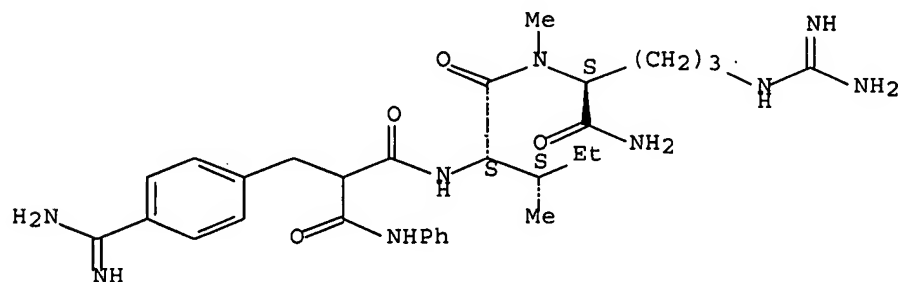
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
β-alanyl-L-isoleucyl-N2-methyl-, trifluoroacetate (9CI) (CA INDEX
NAME)

CM 1

CRN 356543-50-5

CMF C30 H43 N9 O4

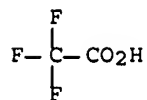
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356543-57-2 CAPLUS

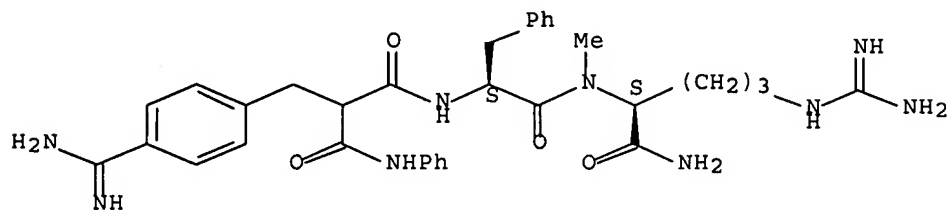
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl- β -alanyl-L-phenylalanyl-N²-methyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356543-56-1

CMF C33 H41 N9 O4

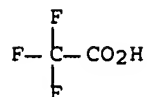
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356543-69-6 CAPLUS

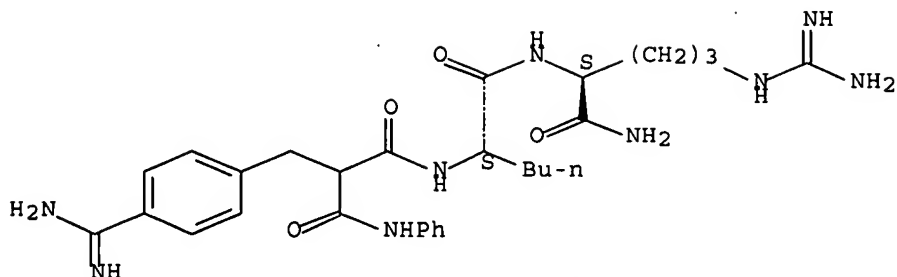
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl- β -alanyl-L-norleucyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356543-68-5

CMF C29 H41 N9 O4

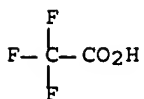
Absolute stereochemistry.



CM 2

CRN 76-05-1

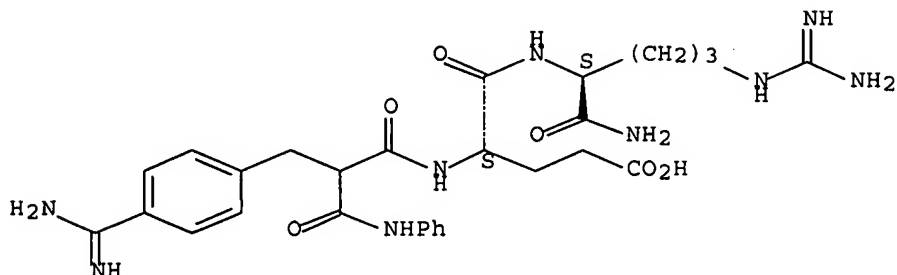
CMF C2 H F3 O2



RN 356543-75-4 CAPLUS

CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
β-alanyl-L-α-glutamyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



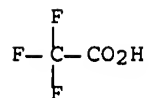
RN 356543-83-4 CAPLUS

CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
β-alanyl-3-(2-naphthalenyl)-L-alanyl-, trifluoroacetate (9CI) (CA
INDEX NAME)

CRN 356543-82-3
CMF C36 H41 N9 O4

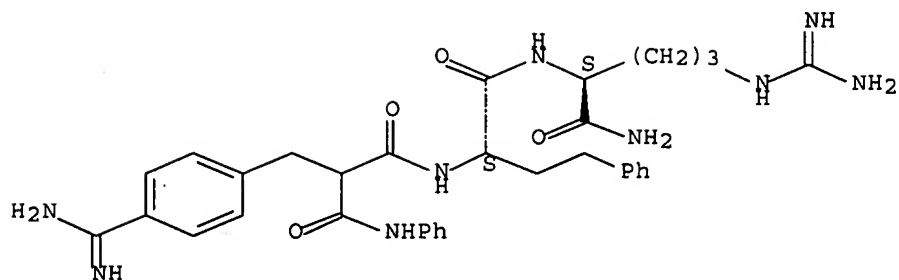
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CRN 76-05-1
CMF C2 H F3 O2



CRN 356543-90-3
CMF C33 H41 N9 O4

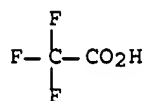
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356543-99-2 CAPLUS

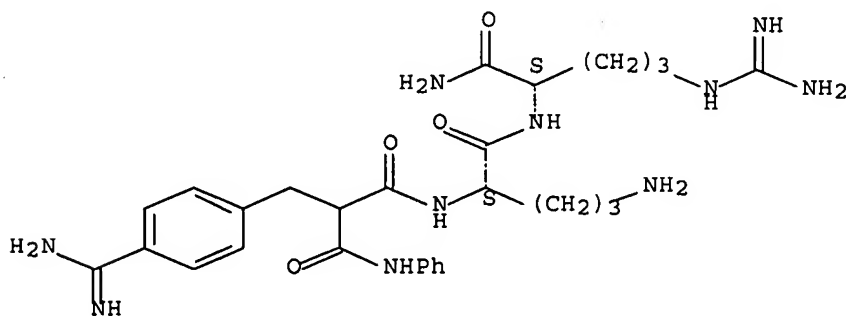
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-beta-alanyl-L-ornithyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356543-98-1

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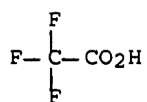
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



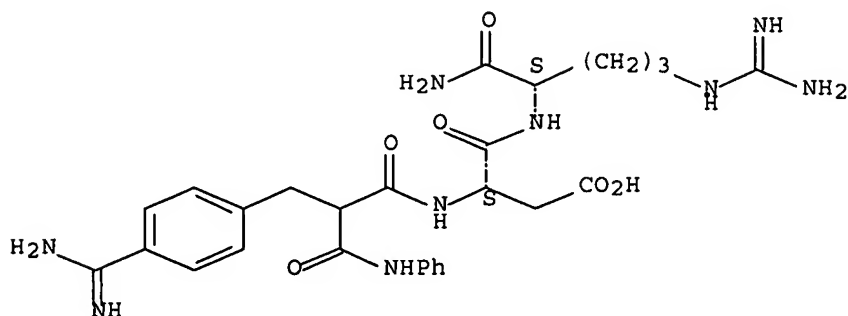
RN 356544-07-5 CAPLUS
 CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
 β-alanyl-L-α-aspartyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356544-06-4

CMF C27 H35 N9 O6

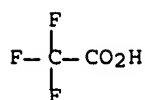
Absolute stereochemistry.



CM 2

CRN 76-05-1

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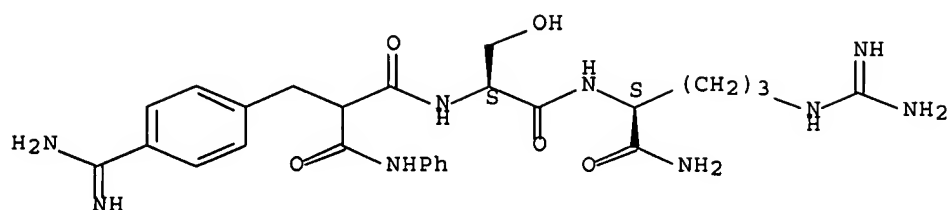
RN 356544-15-5 CAPLUS
 CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
 β-alanyl-L-seryl-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 356544-14-4

CMF C26 H35 N9 O5

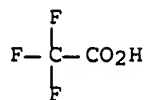
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356544-24-6 CAPLUS

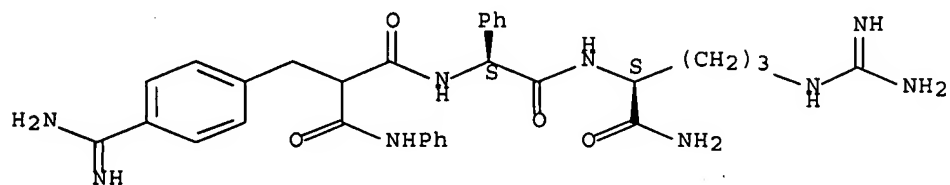
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl- β -alanyl-(2S)-2-phenylglycyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356544-23-5

CMF C31 H37 N9 O4

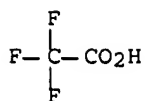
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356544-32-6 CAPLUS

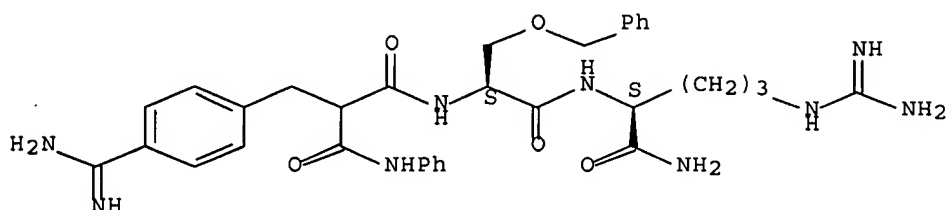
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
β-alanyl-O-(phenylmethyl)-L-seryl-, trifluoroacetate (9CI) (CA INDEX
NAME)

CM 1

CRN 356544-31-5

CMF C33 H41 N9 O5

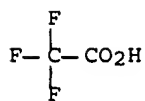
Absolute stereochemistry.



CM 2

CRN 76-05-1

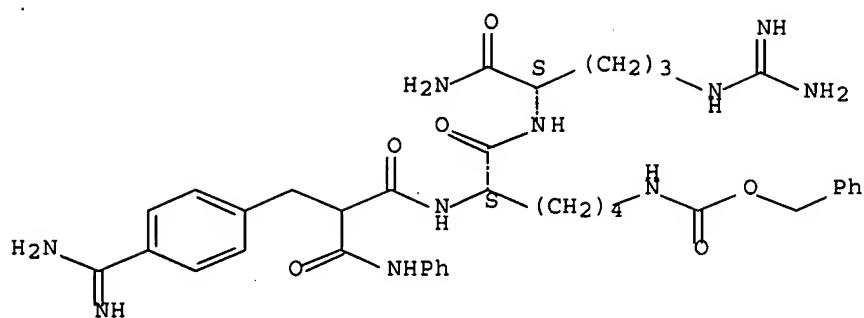
CMF C2 H F3 O2



RN 356544-36-0 CAPLUS

CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
β-alanyl-N6-[(phenylmethoxy)carbonyl]-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 356544-52-0 CAPLUS

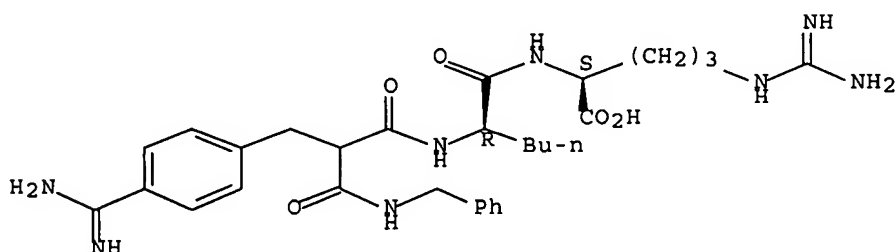
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-D-norleucyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356544-51-9

CMF C30 H42 N8 O5

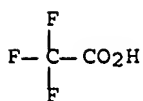
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



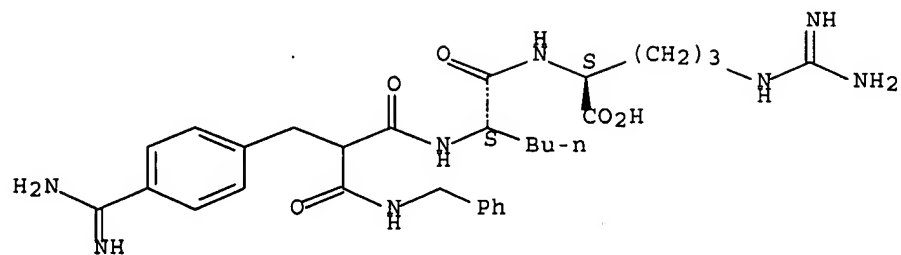
RN 356544-62-2 CAPLUS

CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-L-norleucyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

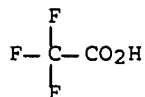
CRN 356544-61-1
CMF C30 H42 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

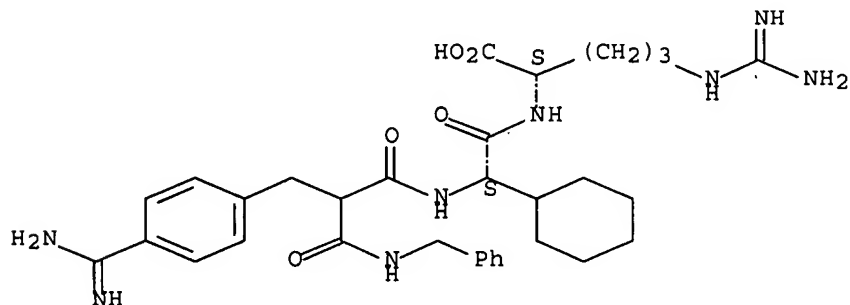


RN 356544-68-8 CAPLUS
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-
β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (9CI) (CA INDEX
NAME)

CM 1

CRN 356544-67-7
CMF C32 H44 N8 O5

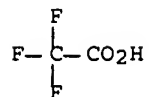
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356544-74-6 CAPLUS

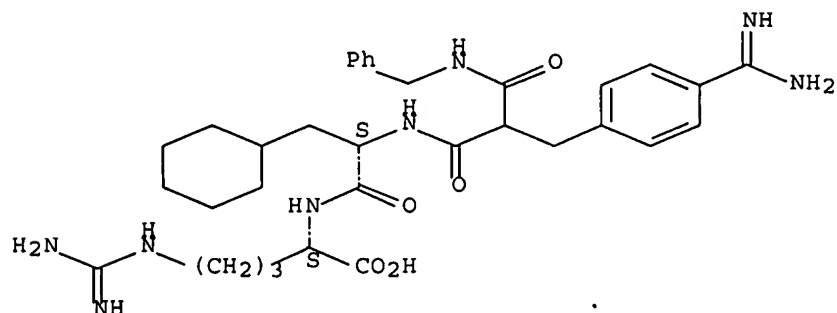
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-
β-alanyl-3-cyclohexyl-L-alanyl-, trifluoroacetate (9CI) (CA INDEX
NAME)

CM 1

CRN 356544-73-5

CMF C33 H46 N8 O5

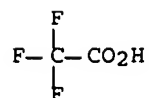
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356544-80-4 CAPLUS

CN Cyclohexanebutanamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-

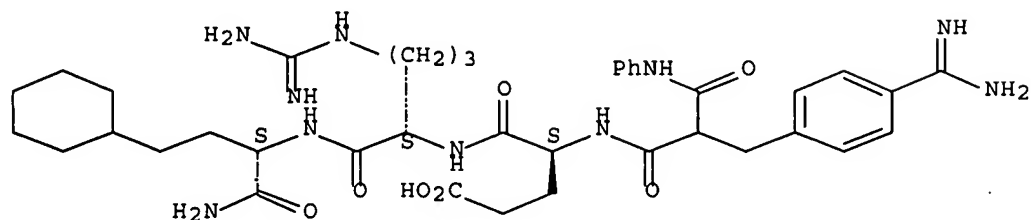
phenyl-β-alanyl-L-α-glutamyl-L-arginyl-α-amino-,
(αS)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356544-79-1

CMF C38 H54 N10 O7

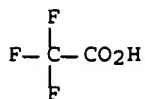
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356545-29-4 CAPLUS

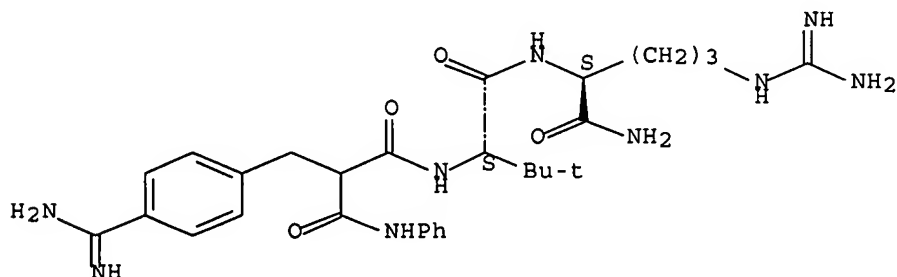
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-β-alanyl-3-methyl-L-valyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

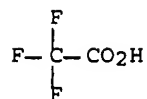
CRN 356545-28-3

CMF C29 H41 N9 O4

Absolute stereochemistry.



CRN 76-05-1
CMF C2 H F3 O2

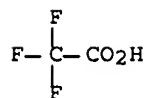


CM 1

CRN 356545-34-1
CMF C31 H43 N9 O4

N#NC(=O)Cc1ccc(cc1)C(Cc2ccccc2N)C(=O)NS(=O)(=O)SC3CCCCC3

CRN 76-05-1
CMF C2 H F3 O2

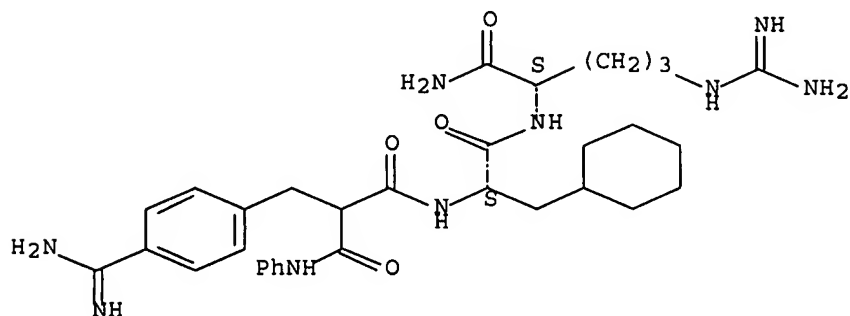


RN 356545-43-2 CAPLUS
 CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-phenyl-
 β -alanyl-3-cyclohexyl-L-alanyl-, trifluoroacetate (9CI) (CA INDEX
 NAME)

CM 1

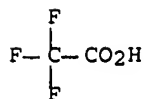
CRN 356545-42-1
 CMF C32 H45 N9 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

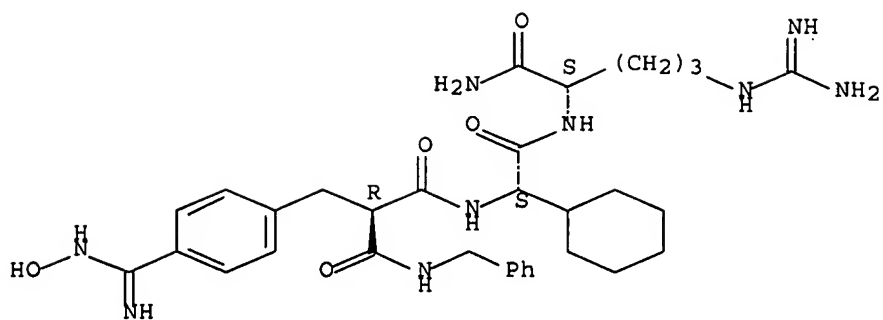


RN 356545-45-4 CAPLUS
 CN L-Argininamide, (2R)-2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-oxo-
 N-(phenylmethyl)- β -alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate
 (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 356545-44-3
 CMF C32 H45 N9 O5

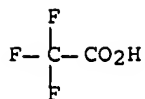
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356545-47-6 CAPLUS

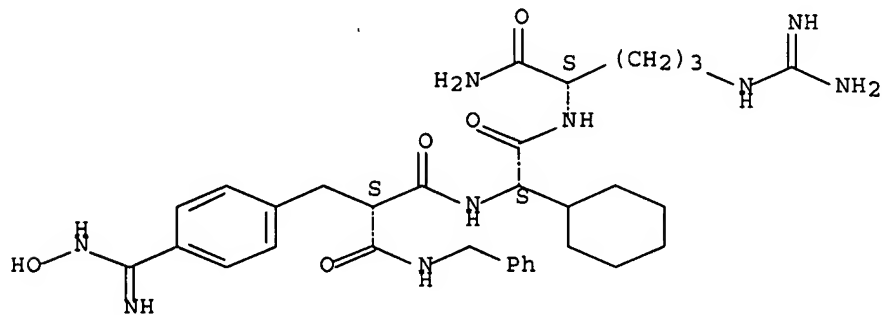
CN L-Argininamide, (2S)-2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 356545-46-5

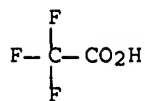
CMF C32 H45 N9 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

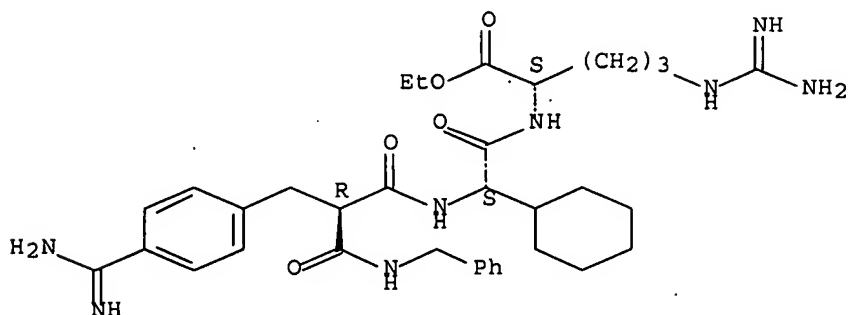


RN 356545-53-4 CAPLUS
CN L-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, ethyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

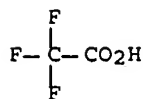
CRN 356545-52-3
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



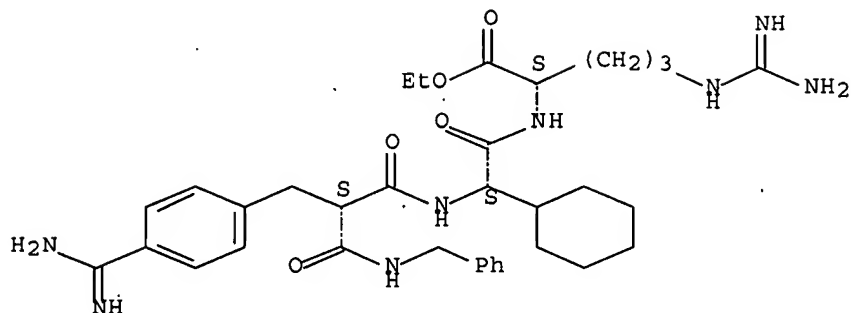
RN 356545-55-6 CAPLUS
CN L-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, ethyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-54-5

CMF C34 H48 N8 O5

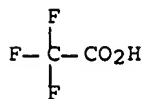
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356545-60-3 CAPLUS

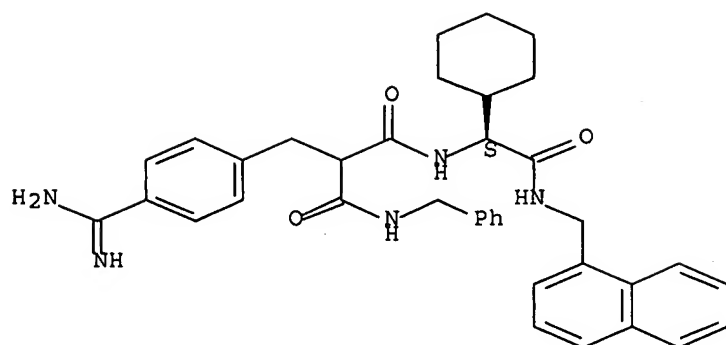
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-[(1-naphthalenylmethyl)amino]-2-oxoethyl]-N'-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-59-0

CMF C37 H41 N5 O3

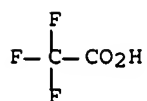
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356545-66-9 CAPLUS

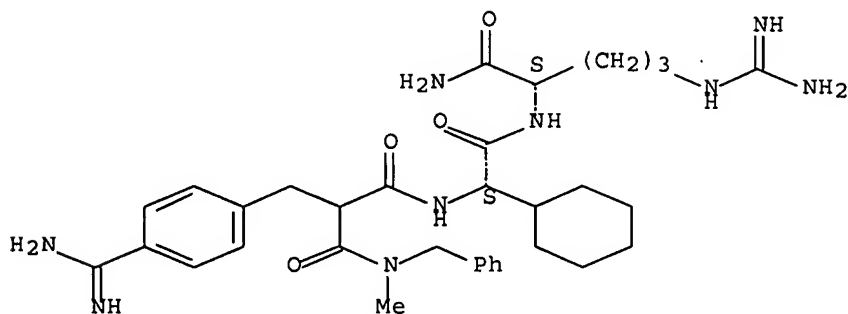
CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, trifluoroacetate
(9CI) (CA INDEX NAME)

CM 1

CRN 356545-65-8

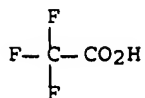
CMF C33 H47 N9 O4

Absolute stereochemistry.



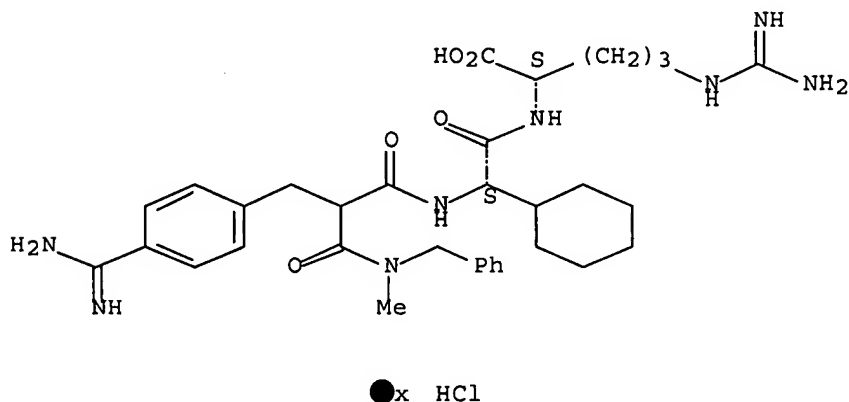
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 356545-67-0 CAPLUS
CN L-Arginine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, hydrochloride (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

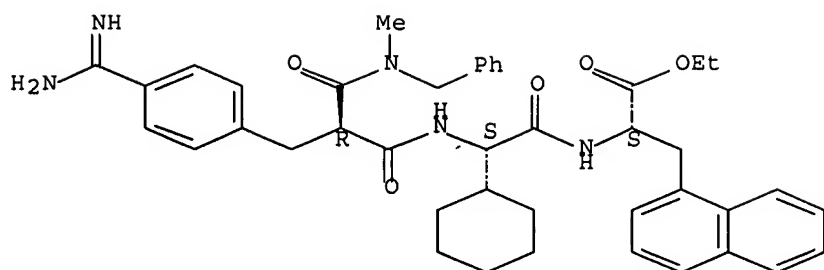


RN 356545-69-2 CAPLUS
CN L-Alanine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 356545-68-1
CMF C42 H49 N5 O5

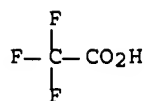
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356545-71-6 CAPLUS

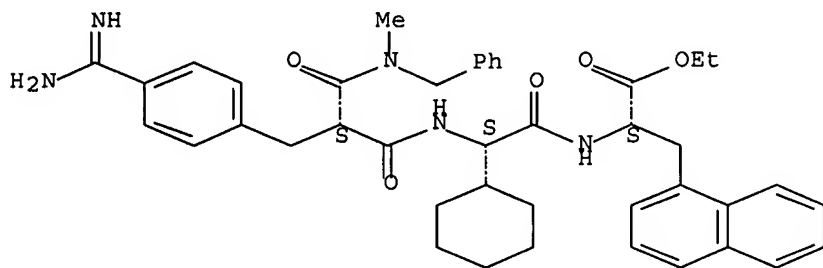
CN L-Alanine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 356545-70-5

CMF C42 H49 N5 O5

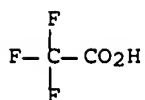
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2

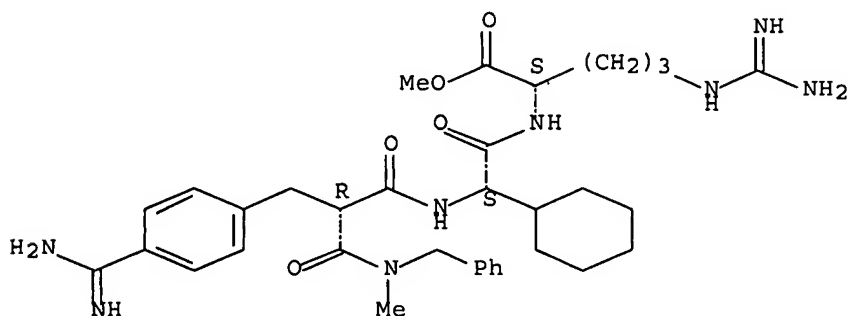


RN 356545-73-8 CAPLUS
 CN L-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

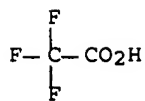
CRN 356545-72-7
 CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

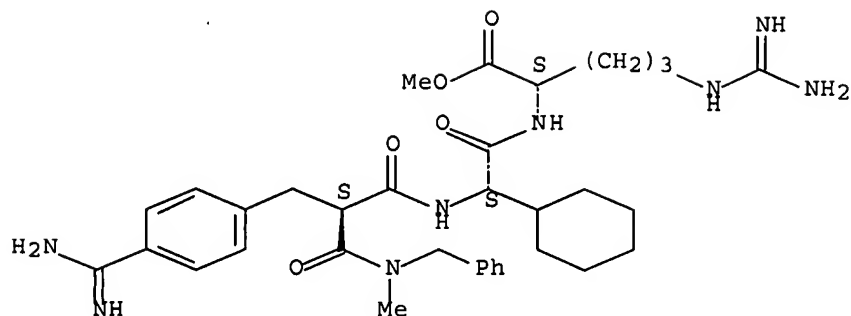


RN 356545-75-0 CAPLUS
 CN L-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

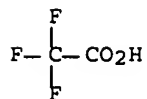
CRN 356545-74-9
CMF C34 H48 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

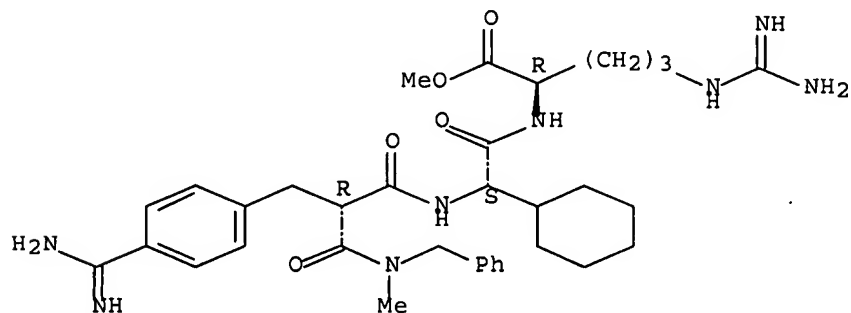


RN 356545-77-2 CAPLUS
CN D-Arginine, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-76-1
CMF C34 H48 N8 O5

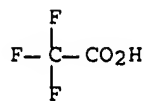
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356545-79-4 CAPLUS

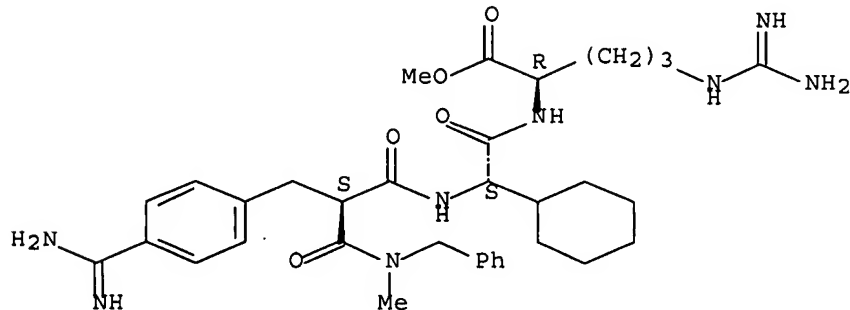
CN D-Arginine, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-, methyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-78-3

CMF C34 H48 N8 O5

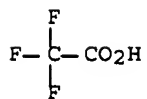
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



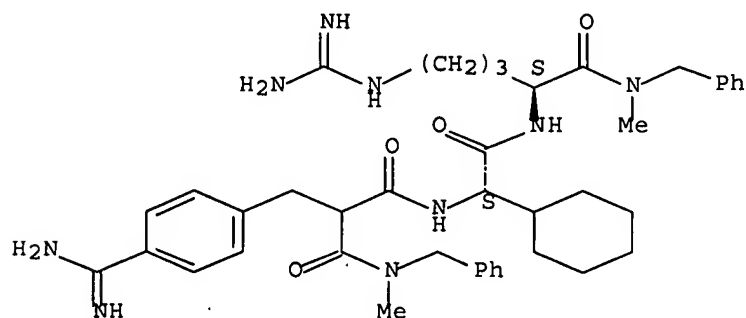
RN 356545-81-8 CAPLUS
 CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-N-methyl-N-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-80-7

CMF C41 H55 N9 O4

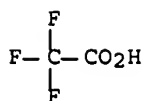
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



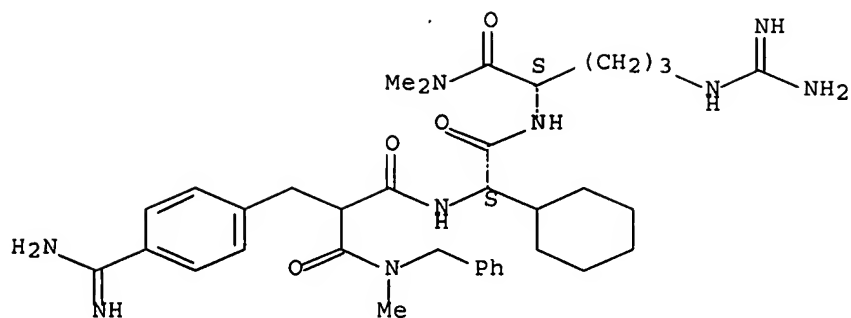
RN 356545-83-0 CAPLUS
 CN L-Argininamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-N,N-dimethyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-82-9

CMF C35 H51 N9 O4

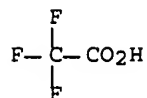
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 356545-85-2 CAPLUS

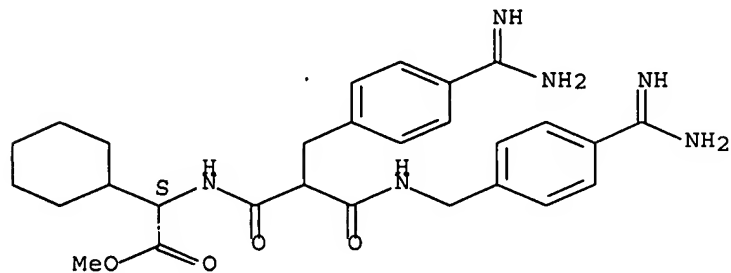
CN Cyclohexaneacetic acid, α -[[2-[[4-(aminoiminomethyl)phenyl]methyl]-3-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1,3-dioxopropyl]amino]-, methyl ester, (α S)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 356545-84-1

CMF C28 H36 N6 O4

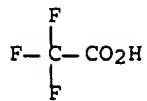
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT 280554-59-8P 280554-60-1P 280554-61-2P

356545-90-9P 356545-91-0P 356545-92-1P

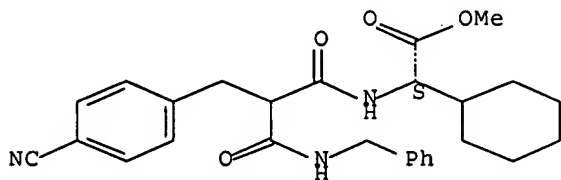
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of malonic acid amide derivs. as inhibitors of blood clotting factor Xa)

RN 280554-59-8 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[(4-cyanophenyl)methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

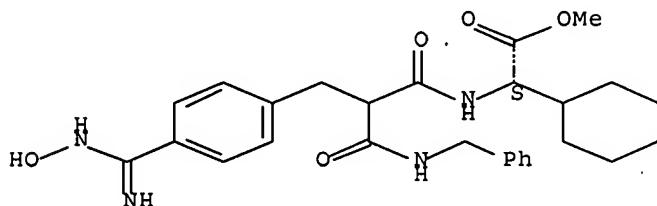
Absolute stereochemistry.



RN 280554-60-1 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

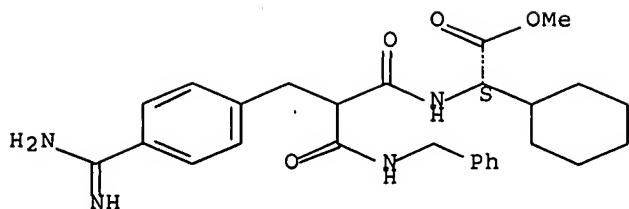
Absolute stereochemistry.



RN 280554-61-2 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

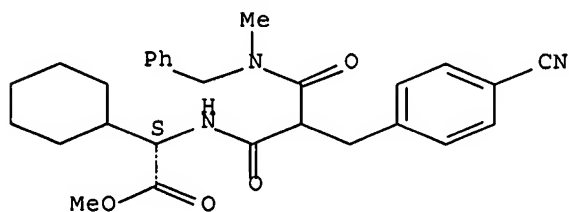
Absolute stereochemistry.



RN 356545-90-9 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-(4-cyanophenyl)methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

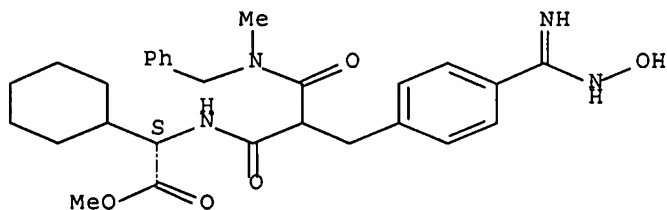
Absolute stereochemistry.



RN 356545-91-0 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (α S)- (9CI) (CA INDEX NAME)

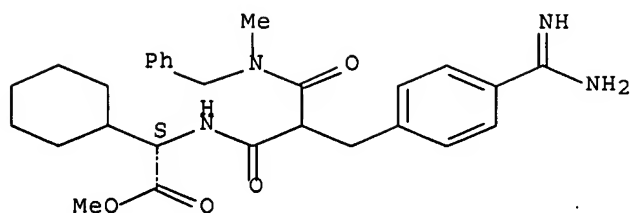
Absolute stereochemistry.



RN 356545-92-1 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-(aminoiminomethyl)phenyl]methyl]-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-, methyl ester, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 10 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:457054 CAPLUS Full-text

DOCUMENT NUMBER: 135:210602

TITLE: Versatile synthesis of malonamic acid derivatives from a β -ketothioester

AUTHOR(S): Lopez-Alvarado, P.; Avendano, C.; Carlos Menendez, J.

CORPORATE SOURCE: Facultad de Farmacia, Departamento de Quimica Organica y Farmaceutica, Universidad Complutense, Madrid, 28040, Spain

SOURCE: Tetrahedron Letters (2001), 42(27), 4479-4482

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:210602

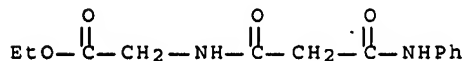
AB An efficient synthetic route is described that allows the preparation under mild conditions of several types of malonamic acid derivs. The S-tert-Bu acetothioacetate monoanion reacted with aryl or alkyl isocyanates to give β -amidothioesters in one step and 73-87% yield, after spontaneous deacetylation of tricarbonyl intermediates. E.g., S-tert-Bu 3-oxothiobutanoate was reacted with cyclohexyl isocyanate to give S-tert-Bu cyclohexylcarbamoylthioacetate in 87% yield. Treatment of these thioesters with several aliphatic or aromatic alcs. and amines at room temperature in THF or DME and in the presence of silver trifluoroacetate provided, resp., the corresponding malonamic acid esters and malonamides in 80-100% yield.

IT 339274-38-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 339274-38-3 CAPLUS

CN Glycine, 3-oxo-N-phenyl- β -alanyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

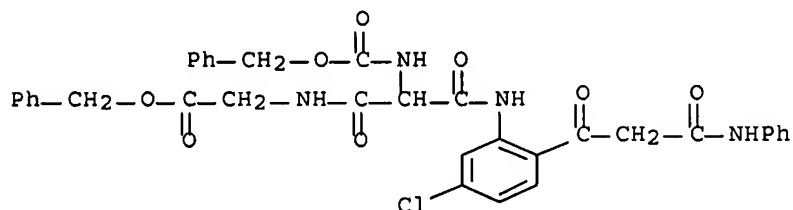
L53 ANSWER 11 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:278994 CAPLUS Full-text

DOCUMENT NUMBER: 135:107312

TITLE: Efficient synthesis of novel benzo-[e]-[1,4]-diazepine

derivatives
 AUTHOR(S): Messeri, T.; Pentassuglia, G.; Di Fabio, R.
 CORPORATE SOURCE: Medicines Research Center, GlaxoWellcome S.p.A.,
 Verona, I-37135, Italy
 SOURCE: Tetrahedron Letters (2001), 42(18), 3227-3230
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:107312
 AB Following two efficient synthetic routes, a novel series of (2Z)-(8-chloro-1,2,3,4-tetrahydro-2-oxo-5H-1,4-benzodiazepin-5-ylidene)-N-phenylacetamide derivs. (bearing an unusual Z exo-methylencarbamoyl side chain at the C-5 position) were prepared to identify new antagonists of the glycine binding site associated with NMDA receptor. Pharmacol. test data were not reported.
 IT 350238-05-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of (2Z)-(8-chloro-1,2,3,4-tetrahydro-2-oxo-5H-1,4-benzodiazepin-5-ylidene)-N-phenylacetamide derivs.)
 RN 350238-05-0 CAPLUS
 CN Glycine, 3-[5-chloro-2-[1,3-dioxo-3-(phenylamino)propyl]phenyl]amino]-3-oxo-N-[(phenylmethoxy)carbonyl]alanyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 12 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:133356 CAPLUS Full-text
 DOCUMENT NUMBER: 134:352962
 TITLE: A general, high-yielding synthesis of β -diamides and β -amido esters
 AUTHOR(S): Lopez-Alvarado, Pilar; Avendano, Carmen; Menendez, J. Carlos
 CORPORATE SOURCE: Departamento de Quimica Organica y Farmaceutica, Facultad de Farmacia, Universidad Complutense, Madrid, 28040, Spain
 SOURCE: Proceedings of ECSOC-3, [and] Proceedings of ECSOC-4, Sept. 1-30, 1999 and 2000 (2000), Meeting Date 1999-2000, 751-754. Editor(s): Pombo-Villar, Esteban. Molecular Diversity Preservation International: Basel, Switz.
 CODEN: 69AXZT
 DOCUMENT TYPE: Conference; (computer optical disk)
 LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:352962

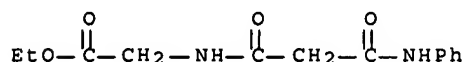
AB An electronic conference report on a new and efficient synthetic route to malonamides and malonamic acid esters. S-tert-Bu acetothioacetate monoanion reacted with aryl or alkyl isocyanates to give tricarbonyl compds., which spontaneously deacetylated to the corresponding β -amido thioesters. Treatment of the latter with aliphatic or aromatic amines or alcs. at room temperature in the presence of silver trifluoroacetate provided malonamides or malonamic acid esters, resp., in excellent overall yields.

IT 339274-38-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of β -diamides and β -amido esters)

RN 339274-38-3 CAPLUS

CN Glycine, 3-oxo-N-phenyl- β -alanyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 13 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:653161 CAPLUS Full-text

DOCUMENT NUMBER: 134:5141

TITLE: Replacement of glycine with dicarbonyl and related moieties in analogs of the C-terminal pentapeptide of cholecystokinin: CCK2 agonists displaying a novel binding mode

AUTHOR(S): Bellier, Bruno; Million, Marie-Emmanuelle; DaNascimento, Sophie; Meudal, Herve; Kellou, Safia; Maigret, Bernard; Garbay, Christiane

CORPORATE SOURCE: Departement de Pharmacochimie Moleculaire et Structurale, U266 INSERM UMR 8600 CNRS, UFR des Sciences Pharmaceutiques et Biologiques, Paris, 75270, Fr.

SOURCE: Journal of Medicinal Chemistry (2000), 43(20), 3614-3623

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:5141

AB Recent advances in the field of cholecystokinin have indicated the possible occurrence of multiple affinity states of the CCK2 receptor. Besides, numerous pharmacol. expts. performed "in vitro" and "in vivo" support the eventuality of different pharmacol. profiles associated to CCK2 ligands. Indeed, some agonists are essentially anxiogenic and ineffective in memory tests, whereas others are not anxiogenic and appear as able to reinforce memory. The reference compound for the latter profile is the CCK-8 analog BC 264 (Boc-Tyr(SO₃H)-gNle-mGly-Trp-(NMe)Nle-Asp-Phe-NH₂). However, although tetrapeptide ligands based on CCK-4 (Trp-Met-Asp-Phe-NH₂) are known to possess sufficient structural features for CCK2 recognition, none shares the properties of BC 264. Hence we have developed new short peptidic or pseudo-peptidic derivs. containing the C-terminal tetrapeptide of BC 264. Our results indicate that some compds. characterized by the presence of two carbonyl groups at the N-terminus, as in (HO₂C-CH₂-CONH-Trp-(NMe)Nle-Asp-Phe-NH₂), are likely to show a

BC 264-like profile, bind to the CCK2 receptor in a specific way, and display remarkable affinities (0.28 nM on guinea-pig cortex membrane preps.). This original binding mode is discussed and further enlightened by NMR and mol. modeling studies.

IT 203563-93-3P

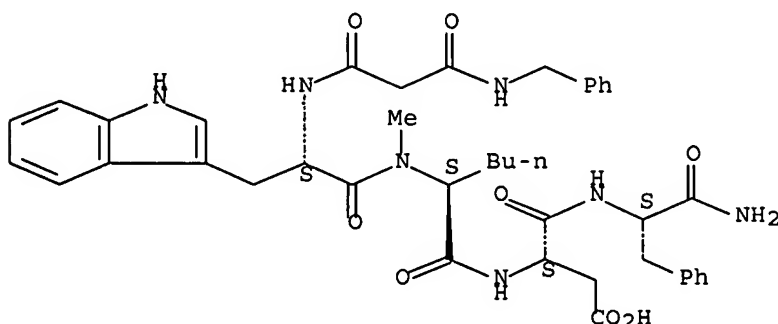
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of pseudopeptides as CCK2 agonists by replacement of glycine with dicarbonyl in C-terminal pentapeptides)

RN 203563-93-3 CAPLUS

CN L-Phenylalaninamide, 3-oxo-N-(phenylmethyl)- β -alanyl-L-tryptophyl-N-methyl-L-norleucyl-L- α -aspartyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 14 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:456736 CAPLUS Full-text

DOCUMENT NUMBER: 133:89228

TITLE: Novel malonic acid derivatives, processes for their preparation, their use and pharmaceutical compositions containing them (inhibition of factor Xa activity)

INVENTOR(S): Defossa, Elisabeth; Heinelt, Uwe; Klingler, Otmar; Zoller, Gerhard; Matter, Hans; Al-Obeidi, Fahad A.; Walser, Armin; Wildgoose, Peter

PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany

SOURCE: Eur. Pat. Appl., 76 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1016663	A1	20000705	EP 1999-100002	19990102
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2358578	A1	20000713	CA 1999-2358578	19991223
WO 2000040571	A1	20000713	WO 1999-EP10340	19991223
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,				

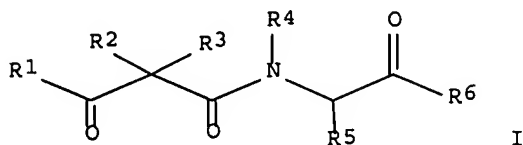
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 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG.

BR 9916732	A	20010925	BR 1999-16732	19991223
EP 1140878	A1	20011010	EP 1999-964667	19991223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200101903	T2	20011121	TR 2001-200101903	19991223
HU 200105437	A2	20020529	HU 2001-5437	19991223
JP 2002534420	T	20021015	JP 2000-592279	19991223
US 6395737	B1	20020528	US 1999-473053	19991228
ZA 2001004770	A	20020612	ZA 2001-4770	20010612
NO 2001002983	A	20010615	NO 2001-2983	20010615
IN 2001CN00908	A	20050304	IN 2001-CN908	20010628

PRIORITY APPLN. INFO.:

EP 1999-100002	A	19990102
EP 1999-119537	A	19991001
WO 1999-EP10340	W	19991223

OTHER SOURCE(S): MARPAT 133:89228
 GI



AB The present invention relates to the preparation of new compds. for the inhibition of blood clotting proteins, and more particularly, to malonic acid derivs., I (R1 = organoamino, organoalkoxy, etc.; R2 = H, C1-4 alkyl; R3 = (un)substituted C6-10-aryl-C1-4-alkyl; R4 = H, C1-4-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl-C1-4-alkyl; R5 = H, C1-10-alkyl, C3-7-cycloalkyl, C3-7-cycloalkyl-C1-4-alkyl, C6-10-aryl, C6-10-aryl-C1-4-alkyl, etc.; R4R5 = cyclic hydrocarbyl; R6 = organoalkoxy, organoamino, etc.). Thus, 2-(R,S)-(4-carbamimidoylbenzyl)-N-[(S)-cyclohexyl(piperidin-4-ylcarbamoyl)methyl]-N',N'-dimethylmalonamide acetic acid salt was prepared in several steps starting from 2,2-dimethyl[1,3]dioxane-4,6-dione and 4-formylbenzonitrile. I are inhibitors (activity given) of the blood clotting enzyme factor Xa. The invention also relates to processes for the preparation of I, to methods of inhibiting factor Xa activity and of inhibiting blood clotting, to the use of I in the treatment and prophylaxis of diseases, which can be treated or prevented by the inhibition of factor Xa activity such as thromboembolic diseases, and to the use of the compds. I in the preparation of medicaments to be applied in such diseases. The invention further relates to compns. containing I in admixt. or otherwise in association with an inert carrier, in particular pharmaceutical compns. containing a compound of formula I together with pharmaceutically acceptable carrier substances and auxiliary substances.

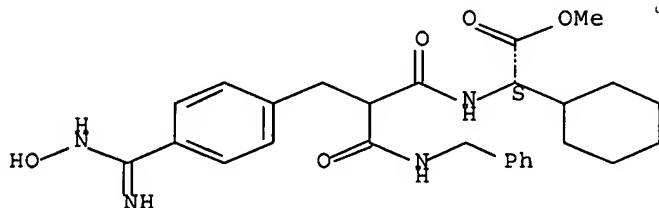
IT 280554-60-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and catalytic hydrogenation of)

RN 280554-60-1 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 280553-84-6P

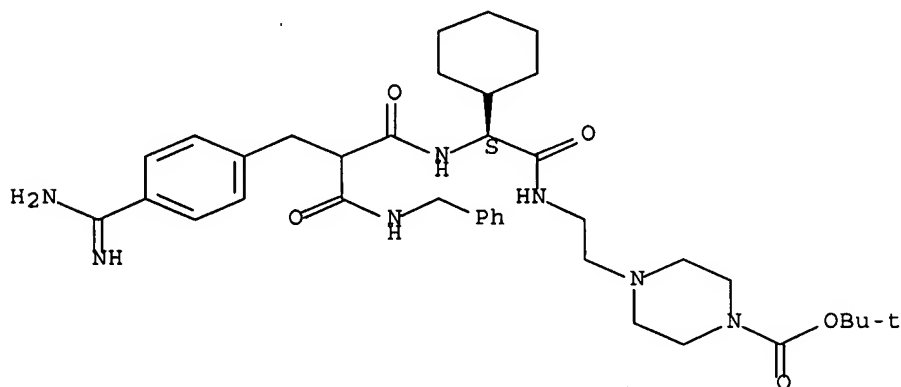
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with benzylcarbamoyl carbamimidoylphenylpropionyl amino cyclohexylacetic acid salt)

RN 280553-84-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-[[[(2S)-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]cyclohexylacetyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 280554-61-2P

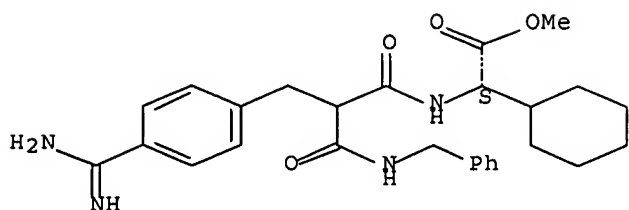
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with hydrochloric acid)

RN 280554-61-2 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

Absolute stereochemistry.



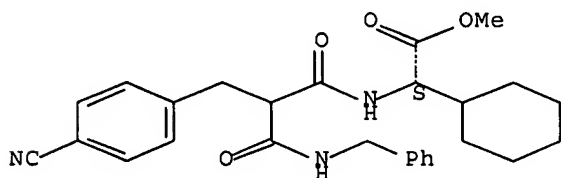
IT 280554-59-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydroxylamine)

RN 280554-59-8 CAPLUS

CN Cyclohexaneacetic acid, α -[[2-[(4-cyanophenyl)methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-, methyl ester, (α S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 280553-85-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of novel malonic acid derivs. as factor Xa inhibitors)

RN 280553-85-7 CAPLUS

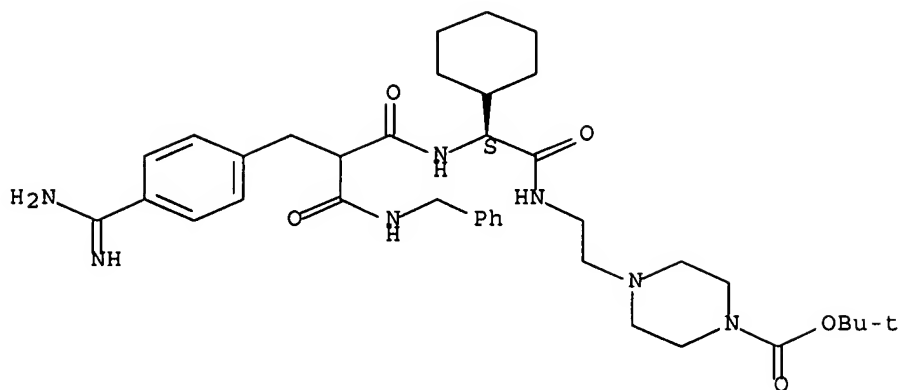
CN 1-Piperazinecarboxylic acid, 4-[2-[[[2S]-[[2-[[[4-(aminoiminomethyl)phenyl]methyl]-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]cyclohexylacetyl]amino]ethyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280553-84-6

CMF C37 H53 N7 O5

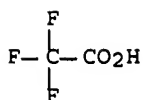
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT 280553-80-2P 280553-83-5P 280553-87-9P
 280553-91-5P 280553-96-0P 280554-05-4P
 280554-06-5P 280554-33-8P 280554-35-0P
 280554-37-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of novel malonic acid derivs. as factor Xa inhibitors)

RN 280553-80-2 CAPLUS

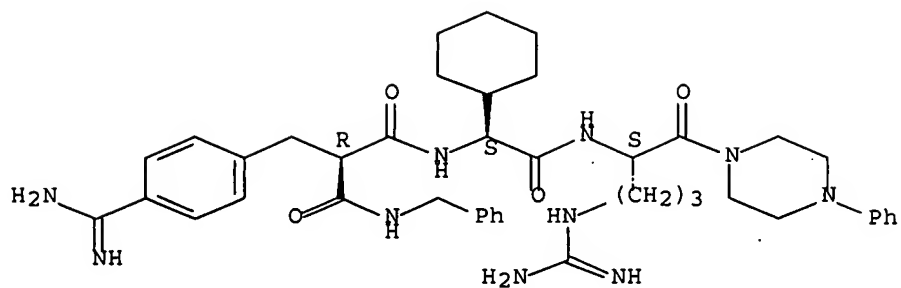
CN Glycinamide, (2R)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280553-79-9

CMF C42 H56 N10 O4

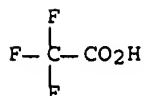
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 280553-83-5 CAPLUS

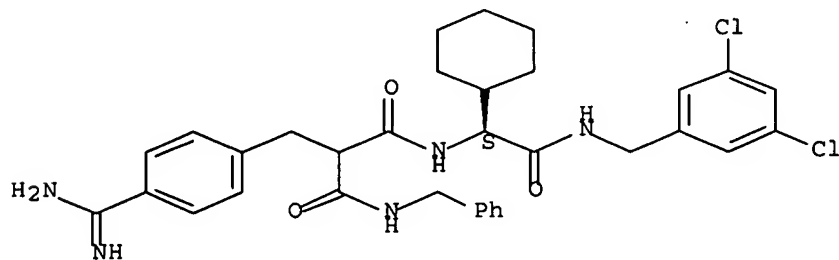
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-[[[(3,5-dichlorophenyl)methyl]amino]-2-oxoethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280553-82-4

CMF C33 H37 Cl2 N5 O3

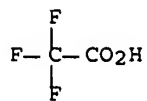
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 280553-87-9 CAPLUS

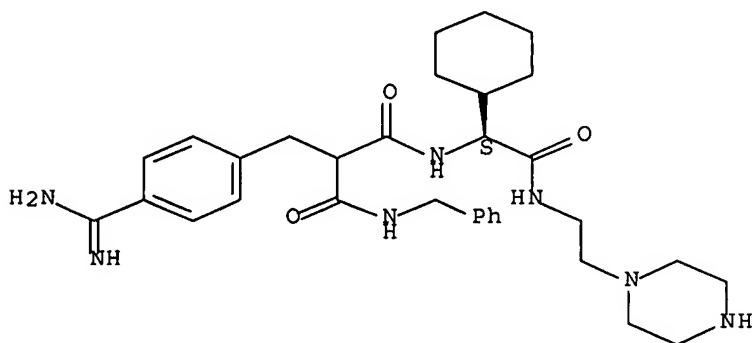
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-1-cyclohexyl-2-oxo-2-[[2-(1-piperazinyl)ethyl]amino]ethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280553-86-8

CMF C32 H45 N7 O3

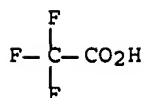
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 280553-91-5 CAPLUS

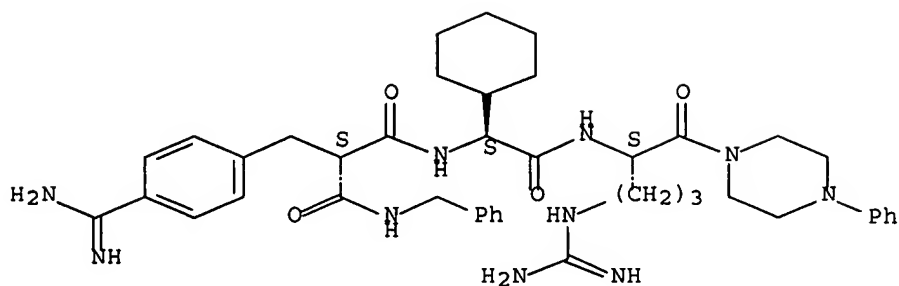
CN Glycinamide, (2S)-2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280553-90-4

CMF C42 H56 N10 O4

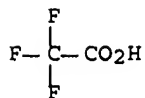
Absolute stereochemistry.



CM 2

CRN 76-05-1

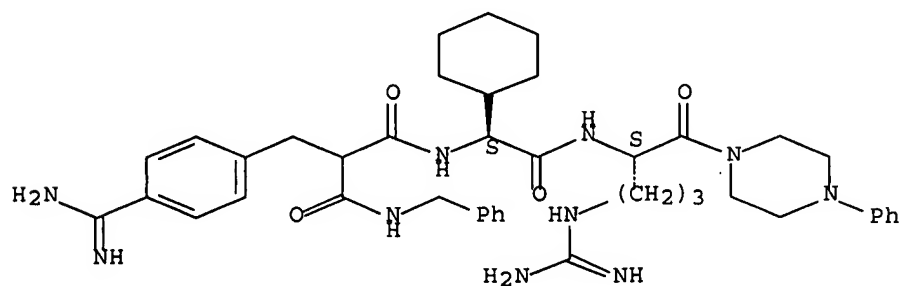
CMF C2 H F3 O2



RN 280553-96-0 CAPLUS

CN Glycinamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-phenyl-1-piperazinyl)carbonyl]butyl]-2-cyclohexyl-, (2S)- (9CI) (CA INDEX NAME)

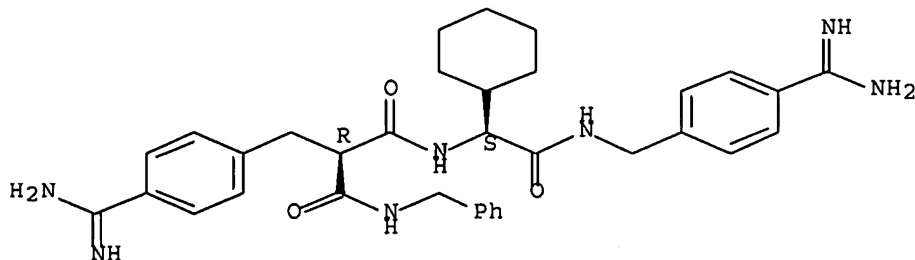
Absolute stereochemistry.



RN 280554-05-4 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-(phenylmethyl)-, (2R)- (9CI) (CA INDEX NAME)

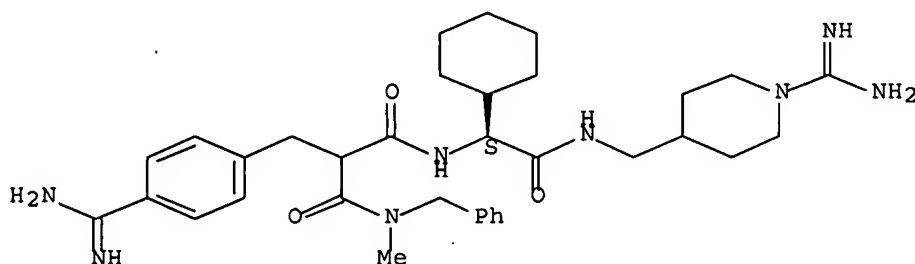
Absolute stereochemistry.



RN 280554-06-5 CAPLUS

CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 280554-33-8 CAPLUS

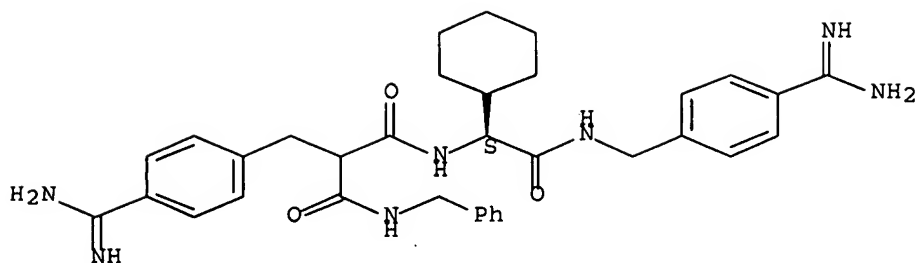
CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-[(1S)-2-[[[4-(aminoiminomethyl)phenyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N'-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280554-32-7

CMF C34 H41 N7 O3

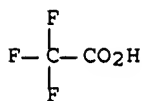
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 280554-35-0 CAPLUS

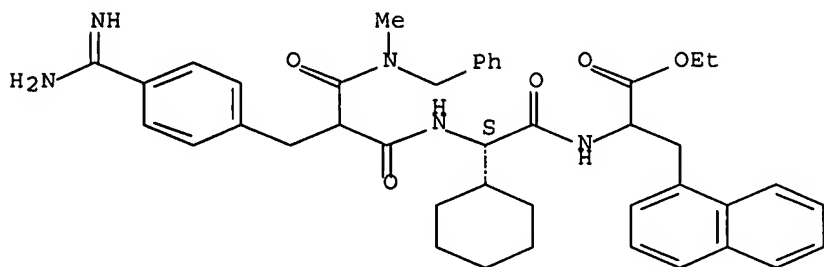
CN Alanine, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N-methyl-3-oxo-N-(phenylmethyl)-β-alanyl-(2S)-2-cyclohexylglycyl-3-(1-naphthalenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 280554-34-9

CMF C42 H49 N5 O5

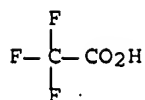
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2

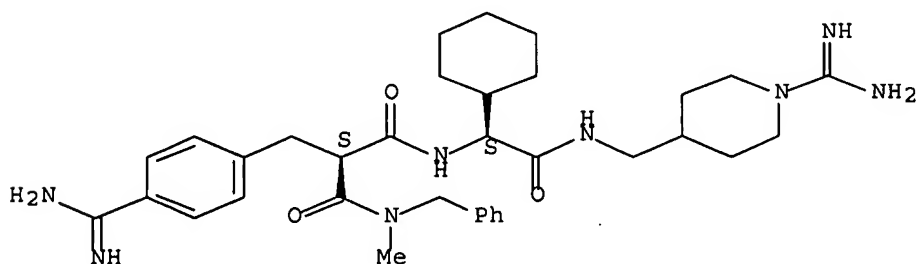


RN 280554-37-2 CAPLUS
 CN Propanediamide, 2-[[4-(aminoiminomethyl)phenyl]methyl]-N'-[(1S)-2-[[[1-(aminoiminomethyl)-4-piperidinyl]methyl]amino]-1-cyclohexyl-2-oxoethyl]-N-methyl-N-(phenylmethyl)-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

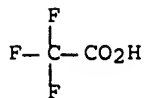
CRN 280554-36-1
 CMF C34 H48 N8 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
 CMF C2 H F3 O2



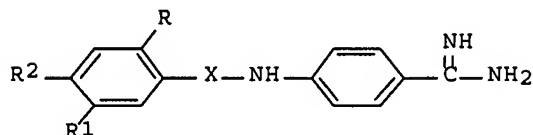
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 15 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:421088 CAPLUS Full-text
 DOCUMENT NUMBER: 133:58615
 TITLE: Substituted aryl and heteroaryl derivatives of benzamidine and their use as antithrombics

INVENTOR(S): Priepke, Henning; Kauffmann, Iris; Huel, Norbert;
 Ries, Uwe; Nar, Herbert; Stassen, Jean Marie; Wienen,
 Wolfgang
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma Kg, Germany
 SOURCE: PCT Int. Appl., 178 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000035859	A1	20000622	WO 1999-EP9921	19991213
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19858029	A1	20000621	DE 1998-19858029	19981216
DE 19948101	A1	20010412	DE 1999-19948101	19991007
CA 2353151	A1	20000622	CA 1999-2353151	19991213
EP 1140802	A1	20011010	EP 1999-965464	19991213
EP 1140802	B1	20040317		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002532460	T	20021002	JP 2000-588121	19991213
JP 3827530	B2	20060927		
AT 261934	T	20040415	AT 1999-965464	19991213
US 6479524	B1	20021112	US 2001-868428	20011018
PRIORITY APPLN. INFO.:				
			DE 1998-19858029	A 19981216
			DE 1999-19948101	A 19991007
			WO 1999-EP9921	W 19991213

OTHER SOURCE(S): MARPAT 133:58615
 GI



AB Aryl and heteroaryl derivs. of benzamidine Ar-A-HCR1-X-Y, such as I [R = Me, H; R1 = CH2CO2Me, Me; R2 = 2-methylpyrrolidinocarbonyl, COCHMe2, N-methyl-N-2-pyridylcarbonyl, pyrrolidinocarbonyl, N(CO2Et)CH2CH2CO2Me, N(CHMe2)NHCH2CO2H, N(CHMe2)COCH2CO2H; X = CH2C.tplbond.C, (CH2)3] were prepared for use as antithrombics. Thus, I [R = Me, R1 = CH2CO2Me, R2 = 2-methylpyrrolidinocarbonyl, X = CH2C.tplbond.C, II] was prepared from the

propargylbenzamidine and pyrrolidinocarbonylphenyl bromide fragments. II had an ED200 in the a-PTT time of 0.23 μ M.

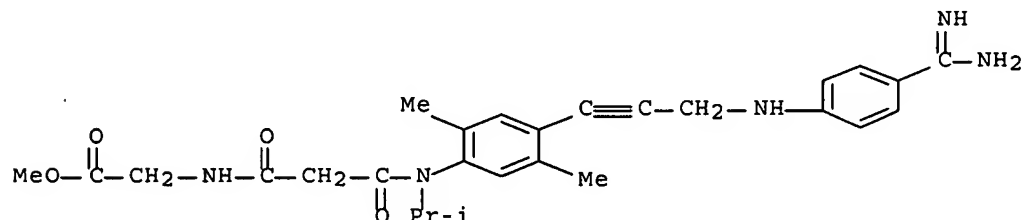
IT 276678-81-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted aryl and heteroaryl derivs. of benzamidine and their use as antithrombics)

RN 276678-81-0 CAPLUS

CN Glycine, N-[4-[3-[[4-(aminoiminomethyl)phenyl]amino]-1-propynyl]-2,5-dimethylphenyl]-N-(1-methylethyl)-3-oxo- β -alanyl-, methyl ester (9CI)
(CA INDEX NAME)



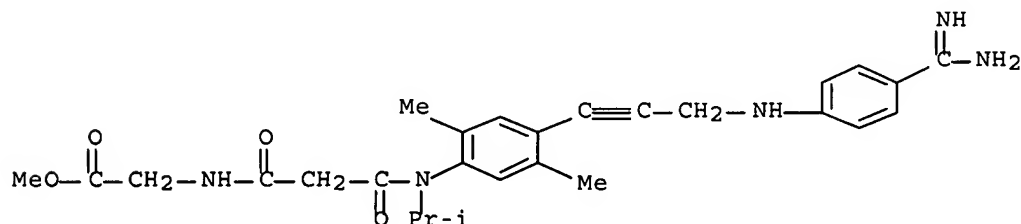
IT 276676-53-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted aryl and heteroaryl derivs. of benzamidine and their use as antithrombics)

RN 276676-53-0 CAPLUS

CN Glycine, N-[4-[3-[[4-(aminoiminomethyl)phenyl]amino]-1-propynyl]-2,5-dimethylphenyl]-N-(1-methylethyl)-3-oxo- β -alanyl-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 16 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:53681 CAPLUS Full-text

DOCUMENT NUMBER: 132:108302

TITLE: Preparation of CS-1 peptidomimetics and their compositions

INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta,

Federico C. A.; He, Ya-Bo; Huyghe, Bernard G.; Chen, Paul G.
 PATENT ASSIGNEE(S): Cytel Corporation, USA
 SOURCE: PCT Int. Appl., 266 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000002903	A1	20000120	WO 1998-US26605	19981215
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9919153	A	20000201	AU 1999-19153	19981215
PRIORITY APPLN. INFO.:			US 1998-113689	A 19980710
			WO 1998-US26605	W 19981215

OTHER SOURCE(S): MARPAT 132:108302

AB Peptidomimetics R1CONR2CHR3CONR4CH(CONR5R6)CH2CO2H [R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, alkyl, phenylalkyl or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl, dialkyl thioether, or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, an optionally substituted 5-, 6-, or 7-membered heterocyclic ring containing 1 or 2 nitrogen atoms, a pyridobenzazepine moiety, or a group CHR7CO-AR8R9 (A = N and R7, R8, R9 = alkyl, a ring structure, etc. or A = O and R7 = alkyl, a ring structure, etc., R8 = alkyl, and R9 is absent)] were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-L-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

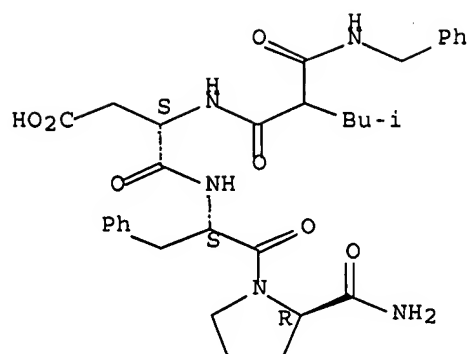
IT 209601-97-8P 209602-44-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of CS-1 peptidomimetics and their compns.)

RN 209601-97-8 CAPLUS

CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-L-α-aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

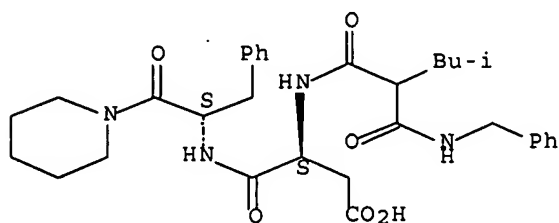
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L- α -Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)- β -alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 17 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:505686 CAPLUS Full-text

DOCUMENT NUMBER: 131:139496

TITLE: Fibronectin CS-1 peptidomimetics for inhibiting binding of CS-1 to VLA-4 and for treating immunoinflammatory conditions

INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.

PATENT ASSIGNEE(S): Cytel Corporation, USA

SOURCE: U.S., 81 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5936065	A	19990810	US 1995-462424	19950605
CA 2177840	A1	19950615	CA 1994-2177840	19941205
CN 1142832	A	19970212	CN 1994-194969	19941205
US 5688913	A	19971118	US 1995-435286	19950505
US 6117840	A	20000912	US 1997-837154	19970414

US 6103870	A	20000815	US 1997-923026	19970903
PRIORITY APPLN. INFO.:			US 1993-164101	B2 19931206
			US 1994-349024	B2 19941202
			US 1995-435286	A1 19950505

OTHER SOURCE(S): MARPAT 131:139496

AB Peptidomimetic compds. are disclosed that inhibit the binding between the VLA-4 and the fibronectin CS-1 compound. Pharmaceutical compns. containing a contemplated compound and methods for treating immunoinflammatory conditions using the compound are also disclosed.

IT 209601-97-8 209602-44-8

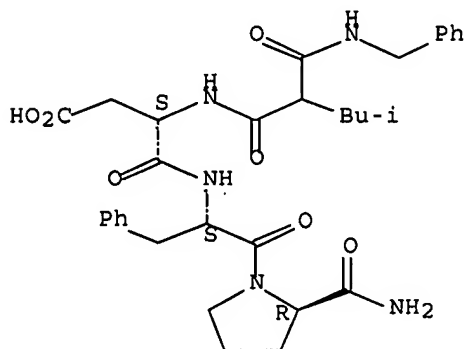
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(fibronectin CS-1 peptidomimetics for inhibiting binding of CS-1 to VLA-4 and for treating immunoinflammatory conditions)

RN 209601-97-8 CAPLUS

CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)- β -alanyl-L- α -aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

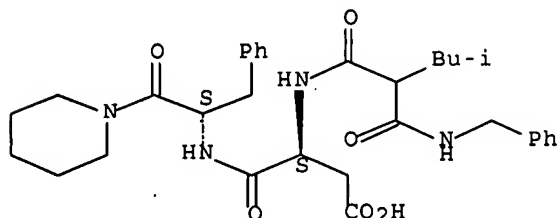
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L- α -Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)- β -alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidiny)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



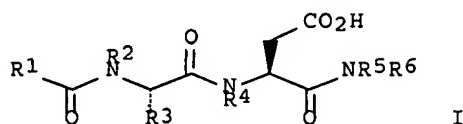
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 18 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:668012 CAPLUS Full-text
 DOCUMENT NUMBER: 129:290438
 TITLE: Preparation of CS-1 peptidomimetics and their compositions
 INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.
 PATENT ASSIGNEE(S): Cytel Corp., USA
 SOURCE: U.S., 81 pp., Cont.-in-part of U.S. Ser. No. 349,024.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5821231	A	19981013	US 1995-461056	19950605
CA 2177840	A1	19950615	CA 1994-2177840	19941205
CN 1142832	A	19970212	CN 1994-194969	19941205
US 5688913	A	19971118	US 1995-435286	19950505
US 6117840	A	20000912	US 1997-837154	19970414
US 6103870	A	20000815	US 1997-923026	19970903
PRIORITY APPLN. INFO.:			US 1993-164101	B2 19931206
			US 1994-349024	A2 19941202
			US 1995-435286	A1 19950505

OTHER SOURCE(S): MARPAT 129:290438
 GI

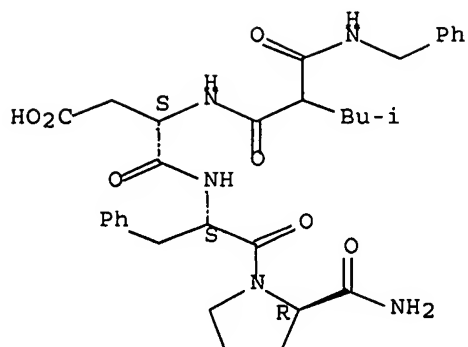


AB Peptidomimetics I (R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, Me or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, 1,1-diphenylmethine, or the R5 ring structure) were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-Leu-Asp-Phe-D-Pro-NH₂ was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

IT 209601-97-8P 209602-44-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of CS-1 peptidomimetics and their compns.)

RN 209601-97-8 CAPLUS
 CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-L-α-aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

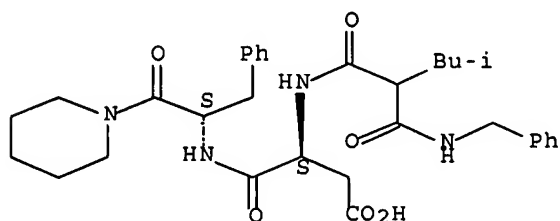
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L-α-Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 19 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:427769 CAPLUS Full-text

DOCUMENT NUMBER: 129:95722

TITLE: Preparation of CS-1 peptidomimetics and their compositions

INVENTOR(S): Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.

PATENT ASSIGNEE(S): Cytel Corp., USA

SOURCE: U.S., 80 pp., Cont.-in-part of U.S. Ser. No. 349,024. CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5770573	A	19980623	US 1995-462219	19950605
CA 2177840	A1	19950615	CA 1994-2177840	19941205
CN 1142832	A	19970212	CN 1994-194969	19941205
US 5688913	A	19971118	US 1995-435286	19950505
US 6117840	A	20000912	US 1997-837154	19970414
US 6103870	A	20000815	US 1997-923026	19970903

PRIORITY APPLN. INFO.:

US 1993-164101

B2 19931206

US 1994-349024

A2 19941202

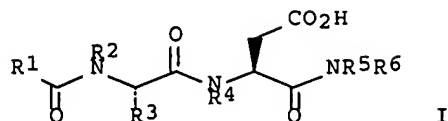
US 1995-435286

A1 19950505

OTHER SOURCE(S):

MARPAT 129:95722

GI



AB Peptidomimetics I (R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, Me or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, 1,1-diphenylmethine, or the R5 ring structure) were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

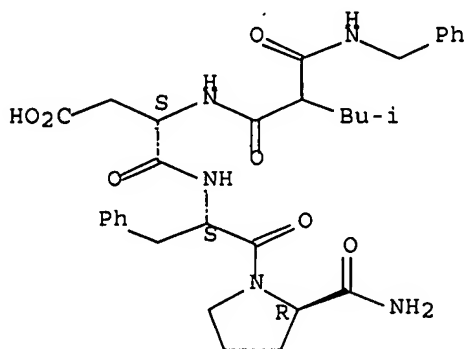
IT 209601-97-8P 209602-44-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of CS-1 peptidomimetics and their compns.)

RN 209601-97-8 CAPLUS

CN D-Prolinamide, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-L-α-aspartyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

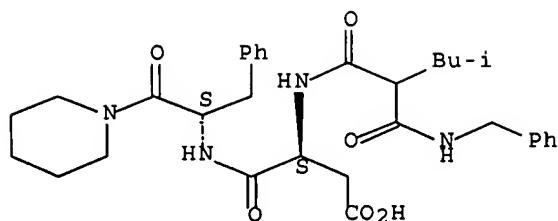
Absolute stereochemistry.



RN 209602-44-8 CAPLUS

CN L-α-Asparagine, 2-(2-methylpropyl)-3-oxo-N-(phenylmethyl)-β-alanyl-N-[(1S)-2-oxo-1-(phenylmethyl)-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 20 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:82115 CAPLUS Full-text

DOCUMENT NUMBER: 128:188696

TITLE: Development of new potent agonists able to interact with two postulated subsites of the cholecystokinin CCK-B receptor

AUTHOR(S): Million, Marie-Emmanuelle; Lena, Isabelle; Da Nascimento, Sophie; Noble, Florence; Dauge, Valerie; Garbay, Christiane; Roques, Bernard Pierre

CORPORATE SOURCE: Dep. Pharmacochimie Moléculaire Structurale, Univ. Rene-Descartes-UFR Scis. Pharmaceutiques Biologiques, Paris, F-75270, Fr.

SOURCE: Letters in Peptide Science (1997), 4(4/5/6), 407-410
CODEN: LPSCEM; ISSN: 0929-5666

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Since the biochem. and pharmacol. profile of BC 197 and BC 264, two CCK8-derived agonists with high specificity for CCK-B receptors, suggests their potential interaction with two CCK-B receptor subsites, it appeared essential to design a new series of compds. that would be able to discriminate between these two subsites. As CCK4 is the shortest fragment of CCK which interacts selectively with CCK-B receptors, compds. derived from the C-terminal tetrapeptide domain of BC 264, Boc-Trp-(NMe)Nle-Asp-Phe-NH₂, and of the cyclic compound BC 197, were prepared While RB 360 (N(cycloamido)- α -Me(R)Trp-[(2S)-2-amino-9-((cycloamido)carbonyl)nonanoyl]-Asp-Phe-NH₂), like BC 197, has a CCK-B1 profile with anxiogenic-like effects in the elevated plus-maze test, RB 400 (HOOC-CH₂-CO-Trp-(NMe)Nle-Asp-Phe-NH₂), like BC 264, seems to be a specific CCK-B2 agonist, able to increase attention and/or memory processes in the Y-maze test.

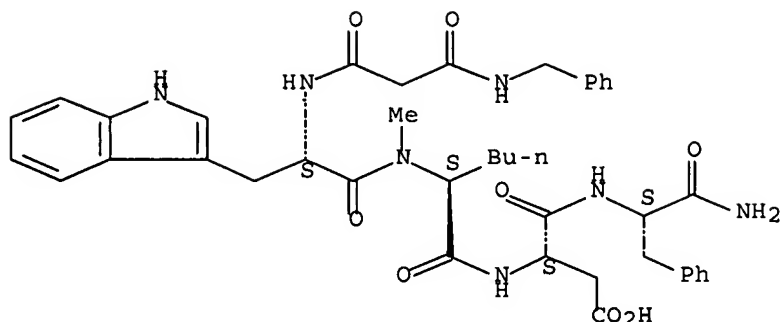
IT 203563-93-3, RB 401

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(development of new potent agonists able to interact with two postulated subsites of cholecystokinin CCK-B receptor)

RN 203563-93-3 CAPLUS

CN L-Phenylalaninamide, 3-oxo-N-(phenylmethyl)- β -alanyl-L-tryptophyl-N-methyl-L-norleucyl-L- α -aspartyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 21 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:740382 CAPLUS Full-text

DOCUMENT NUMBER: 128:359

TITLE: Method for detecting and/or quantifying a hapten in a homogeneous phase using hapten-inhibitor complex, antibody, β -lactamase, and reporter substrate, and device for implementation thereof

INVENTOR(S): Kohl, Michel; Renotte, Roger; Ghitti, Gianangelo; Sarlet, Guy; Lejeune, Robert

PATENT ASSIGNEE(S): Biocode S.A., Belg.; Kohl, Michel; Renotte, Roger; Ghitti, Gianangelo; Sarlet, Guy; Lejeune, Robert

SOURCE: PCT Int. Appl., 67 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9741435	A1	19971106	WO 1997-BE52	19970430
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, DE, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
BE 1010184	A3	19980203	BE 1996-384	19960430
CA 2252931	A1	19971106	CA 1997-2252931	19970430
AU 9726286	A	19971119	AU 1997-26286	19970430
EP 897540	A1	19990224	EP 1997-917955	19970430
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
JP 2000509495	T	20000725	JP 1997-538408	19970430
AT 202848	T	20010715	AT 1997-917955	19970430
US 6436649	B1	20020820	US 1999-171819	19990611
US 2003235877	A1	20031225	US 2002-269673	20021010
PRIORITY APPLN. INFO.:			BE 1996-384	A 19960430
			WO 1997-BE52	W 19970430
			US 1999-171819	A2 19990611
			US 2002-75648	A1 20020213

AB The invention discloses a method for detecting and/or quantifying a hapten (e.g. a drug or hormone) in a homogeneous phase, comprising the following steps: adding a known quantity of a hapten-inhibitor complex to the solution containing the hapten to be detected and/or quantified; adding to the solution a quantity of antibodies corresponding to the quantity of the hapten/inhibitor complex; adding to the solution a type C β -lactamase having an active site for two substrates in antigenic competition in the active site, the first substrate being a reporter substrate capable of being transformed into a detectable and/or quantifiable product, preferably by UV-visible radiation measurement, the second substrate being the hapten/inhibitor complex acting on the hydrolysis rate of the reporter substrate; detecting and/or quantifying the concentration of the product resulting from the transformation of the reporter substrate, the K_m of the reporter substrate being at least a hundred times higher than the K_m of the hapten/inhibitor complex, and the k_{cat} being at least ten times higher than the k_{cat} of the hapten/inhibitor complex. Preparation of reagent conjugates, e.g. nandrolone carbenicillinate, is described, as is determination of e.g. nandrolone.

IT 198830-23-8P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

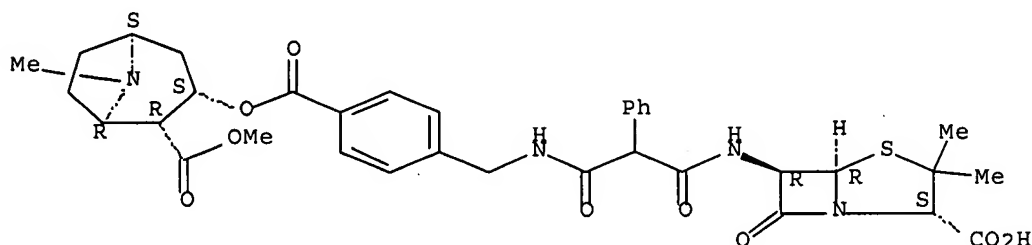
(hapten detection or determination in homogeneous phase using hapten-inhibitor

complex, antibody, β -lactamase, and reporter substrate, implementation device, and reagent preparation)

RN 198830-23-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[[4-[[[3-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]amino]-1,3-dioxo-2-phenylpropyl]amino]methyl]benzoyl]oxy]-8-methyl-, 2-methyl ester, (1R,2R,3S,5S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 22 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:481776 CAPLUS Full-text

DOCUMENT NUMBER: 127:217787

TITLE: Isolation and synthesis of rufulamide, an oligopeptide analog from Metzgeria rufula

AUTHOR(S): Kraut, Ludwig; Klaus, Thomas; Mues, Rudiger; Eicher, Theophil; Zinsmeister, Hans Dietmar

CORPORATE SOURCE: Fachbereich Botanik, Fachbereich Organische Chemie, Univ. Saarlandes, Saarbrücken, D-66041, Germany

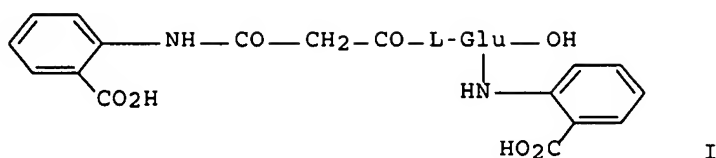
SOURCE: Phytochemistry (1997), 45(8), 1621-1626
CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



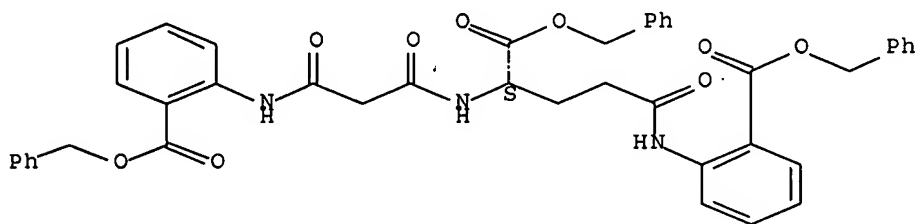
AB An oligopeptide analog, rufulamide (I), consisting of L-glutamic, malonic and 2 mols. of anthranilic acid combined via amide bonds was isolated from the liverwort Metzgeria rufula. Its structure was elucidated by spectroscopic methods and by chemical synthesis.

IT 194875-99-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate in preparation of rufulamide)

RN 194875-99-5 CAPLUS

CN L-Glutamine, 3-oxo-N-[2-[(phenylmethoxy)carbonyl]phenyl]-β-alanyl-N-[2-[(phenylmethoxy)carbonyl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 23 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:462231 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 125:115153

TITLE: Preparation of (acylamino)acetamide derivatives with agonist activity for cholecystokinin-A receptors

INVENTOR(S): Dezube, Milana; Hirst, Gavin Charles; Willson, Timothy Mark; Sherrill, Ronald George; Sugg, Elizabeth Ellen; Szewczyk, Jerzy Ryszard

PATENT ASSIGNEE(S): Glaxo Wellcome Inc., USA

SOURCE: PCT Int. Appl., 121 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

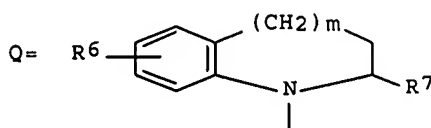
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9611940	A1	19960425	WO 1995-EP4026	19951012

W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM
 RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9538418 A 19960506 AU 1995-38418 19951012
 EP 785944 A1 19970730 EP 1995-936483 19951012
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
 JP 10511929 T 19981117 JP 1995-512935 19951012
 US 5889182 A 19990330 US 1997-817363 19970414

PRIORITY APPLN. INFO.: GB 1994-20763 A 19941014
 WO 1995-EP4026 W 19951012

OTHER SOURCE(S): MARPAT 125:115153
 GI



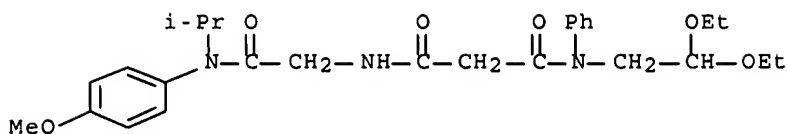
AB A cholecystokinin-A (CCK-A) agonist of the general formula $R_1R_2NCOCH_2NR_3COR_4$ [R1 = C3-6 alkyl, C3-6 cycloalkyl, C3-6 alkenyl, Ph, (CH2)pCN, (CH2)pCO2(C1-4 alkyl); R2 = C3-6 alkyl, C3-6 cycloalkyl, C3-6 alkenyl, PhCH2, Ph or Ph mono- or disubstituted independently with C1-3 alkyl, CN, OH, NMe2, O(C1-4 alkyl), OCH2Ph, NH(C1-4 alkyl), CO2(C1-4 alkyl), N(C1-4 alkyl)2, pyrrolidino, morpholino, halo, C1-3 alkyl substituted by 1 or more F; R1 = C1-2 alkyl, R2 = 2- or 4-C6H4R, R = Cl, Me, MeO, CO2Me; R1R2N = Q; R3 = C1-6 alkyl; Ph or Ph substituted by 1 or 2 C1-3 alkyl, C1-4 alkoxy or halo groups, thiophenyl; R4 = CR6R9(CH2)n(NH)p(CO)q(NH)rR5, CH2N(CHR16R17)CO(NR)rR5; R5 = C1-6 alkyl, C3-8 cycloalkyl, Ph, mono- or disubstituted Ph, optionally substituted heteroaryl or bicycloheteroaryl; R6 = H, optionally substituted C1-3 alkyl; R7 = H, Me; R8 = H, OH, F, NMe2, C1-4 alkoxy, PhCH2O; R9 = H, C1-6 alkyl; R16 = C1-6 alkyl, C3-8 cycloalkyl, optionally halo substituted Ph, pyridyl, pyrimidinyl, thiophenyl; R17 together with R3 form o-disubstituted Ph ring optionally substituted with halo, CF3, C1-3 alkyl, C1-4 alkylthio, of C1-4 alkoxy; m = 0-2; n = 0-3; p = 0, 1; q = 0, 1; r = 0, 1] and physiol. acceptable salts thereof. Thus, ureidodipeptide amide PhNHCO-D-Glu-N(Ph)CH2CON(CHMe2)C6H4OMe-4, prepared in 4 steps from Boc-D-Glu(OCMe3)-OH, PhNH2, and BrCH2CON(CHMe2)C6H4OMe-4, was 55% as active as sulfated CCK-8 in a guinea pig gall bladder assay.

IT 179083-73-9P 179083-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of (acylamino)acetamide derivs. with agonist activity for cholecystokinin-A receptors)

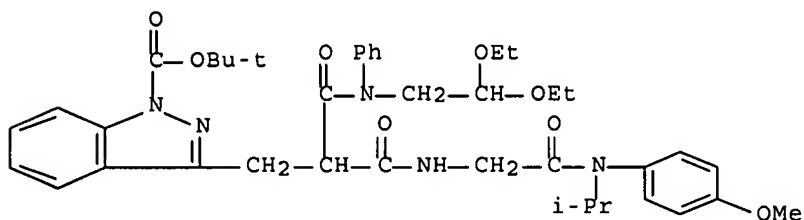
RN 179083-73-9 CAPLUS

CN Glycinamide, N-(2,2-diethoxyethyl)-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 179083-74-0 CAPLUS

CN Glycinamide, N-(2,2-diethoxyethyl)-2-[[1-[(1,1-dimethylethoxy)carbonyl]-1H-indazol-3-yl]methyl]-3-oxo-N-phenyl-β-alanyl-N-(4-methoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



L53 ANSWER 24 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:207549 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 124:279362

TITLE: Inhibition of angiotensin converting enzyme and potentiation of bradykinin by retro-inverso analogs of short peptides and sequences related to angiotensin I and bradykinin

AUTHOR(S): Carmona, Adriana K.; Juliano, Luiz

CORPORATE SOURCE: Dep. Biophysics, Escola Paulista Medicina, Sao Paulo, Brazil

SOURCE: Biochemical Pharmacology (1996), 51(8), 1051-60

CODEN: BCPCA6; ISSN: 0006-2952

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB There is pharmacol. evidence indicating that, in addition to the inhibition of angiotensin converting enzyme (ACE; EC 3.4.15.1), the potentiation of bradykinin (BK) responses may also involve the BK receptor or some binding site in the structures involved in the contractile response to this peptide. Dipeptides such as Val-Trp and some of its analogs as well as tripeptide homologs, including total and partial retro-inverso peptides, were synthesized and assayed for their ability to inhibit purified guinea pig plasma ACE and to potentiate the action of BK on the isolated ileum of the same species. The peptides containing the P2-P1, P1-P'1, and P'1-P'2 inverted amide bonds inhibited ACE, were resistant to hydrolysis, and, depending on the amino acid composition, some of them potentiated the contractile response to BK while others did not. Des-[Arg1]-BK, which has an intrinsic activity at concns. higher than 10⁻⁵M, and the very dissimilar angiotensin I (AI) analog [Cys5-Cys10]-angiotensin-I-(5-10)-amide, which has no detectable contractile activity, were able to inhibit ACE and potentiate BK. In contrast to these peptides, BPP5a and BPP9a from Bothrops jararaca venom, and potentiators B and C from Agkistrodon halys blomhoffi venom were more effective as BK potentiators than as ACE inhibitors. In conclusion, the authors have

synthesized and assayed compds. that preferentially inhibit ACE, e.g. retro-inverso tripeptides, or potentiate the response of smooth muscle to BK, e.g. snake venom peptides.

IT 175412-96-1P

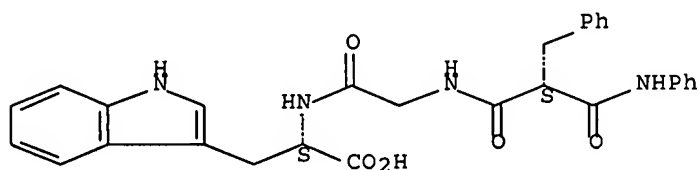
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(angiotensin converting enzyme inhibition and bradykinin potentiation by angiotensin I and bradykinin short peptide retro-inverso analogs)

RN 175412-96-1 CAPLUS

CN L-Tryptophan, N-[N-[3-oxo-N-phenyl-(S)-2-(phenylmethyl)-β-alanyl]glycyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 25 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:828305 CAPLUS Full-text

DOCUMENT NUMBER: 123:228915

TITLE: Preparation of biphenyllyltetrazole-containing amino acid and dipeptide derivatives as angiotensin II antagonists

INVENTOR(S): Naka, Yoichi; Sonda, Shuji; Nakagawa, Haruto; Uehata, Masayoshi

PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

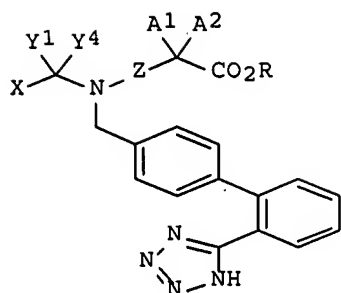
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

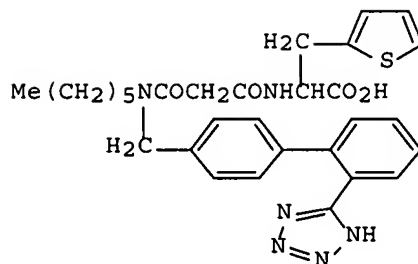
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07048360	A	19950221	JP 1994-116464	19940530
PRIORITY APPLN. INFO.:			JP 1994-116464	A 19940530
			JP 1993-154348	19930531

OTHER SOURCE(S): MARPAT 123:228915

GI



I



II

AB The title compds. [I; X = (un)substituted NH₂, alkenyl, cycloalkyl, aryl, or heteroaryl, saturated carbocyclyl containing NR in the ring; wherein R = H, acyl, alkoxy carbonyl, aralkoxy carbonyl; Y₁, Y₂ = H, alkyl, alkenyl, cycloalkyl, halo, OR₁, NHR₁, CO₂ R₁, CONHR₁, COR₁, aryl, heteroaryl; or Y₁Y₂ = O, S; wherein R₁ = H, alkyl, alkenyl, cycloalkyl, aryl, heteroaryl; Z = CONH, CH₂CONH, COCH₂NH, COCH₂CONH, single bond; when Z = CONH, A₁A₂ = cycloalkane ring optionally having a benzene ring-fused C5-7 substituent; when Z = CH₂CONH, COCH₂NH, COCH₂CONH, or single bond, A₁, A₂ = H, (un)substituted alkyl, alkenyl, cycloalkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl or A₁A₂ = cycloalkane ring optionally having a benzene ring-fused C5-7 substituent], useful for the treatment of hypertension, ischemic heart failure, stroke, kidney diseases, and hypertrophy of the heart or blood vessels, are prepared Thus, H-Phe-OCH₂Ph was alkylated by [2'-(triphenylmethyl-1H-tetrazol-5-yl)biphenyl-4-yl]methyl bromide in the presence of K₂CO₃ in DMF at room temperature for 24 h and then condensed with Z-Pro-Cl in aqueous NaHCO₃/CH₂Cl₂ at room temperature for 3 h followed by deprotection with 2 N HCl/dioxane and hydrogenolysis over 10% Pd-C in EtOH-dioxane to give N-(S)-prolyl-N-[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl-(S)-phenylalanine. (RS)-(2-thienyl)alanine derivative (II) in vitro showed IC₅₀ of 13 nM against angiotensin II in vascular smooth muscle cells of rat thoracic aorta.

IT 168466-38-4P

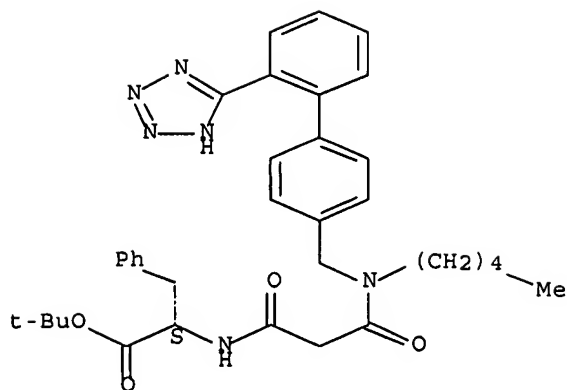
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate for preparation of biphenyltetrazole-containing amino acid and dipeptide derivs. as angiotensin II antagonists)

RN 168466-38-4 CAPLUS

CN L-Phenylalanine, N-[3-oxo-N-pentyl-N-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-β-alanyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 26 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:643894 CAPLUS Full-text

DOCUMENT NUMBER: 123:313504

TITLE: New applications of fluorinated building blocks

AUTHOR(S): Abouabdellah, A.; Boros, L.; Gyenes, F.; Welch, J. T.

CORPORATE SOURCE: Department of Chemistry, State University of New York, Albany, NY, 12222, USA

SOURCE: Journal of Fluorine Chemistry (1995), 72(2), 255-9
CODEN: JFLCAR; ISSN: 0022-1139

PUBLISHER: Elsevier Sequoia

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:313504

AB A new and versatile synthesis of optically active α -fluoromalonamide derivs. from enantiomerically pure 3-fluoro-2-azetidinones is described. A fluorinated retroamide isostere based on these α -fluoromalonamides was introduced into a small peptidomimetic for use as an HIV-1 protease inhibitor. The same strategy was employed in efforts to prepare a novel trifluorostatone-type peptidomimetic.

IT 160000-01-1P

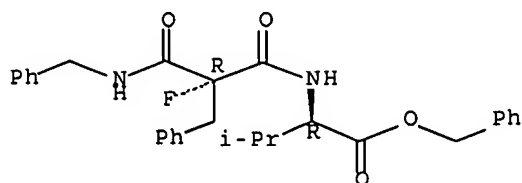
RL: SPN (Synthetic preparation); PREP (Preparation)

(versatile synthesis of optically active α -fluoromalonamide derivs. from enantiomerically pure 3-fluoro-2-azetidinones)

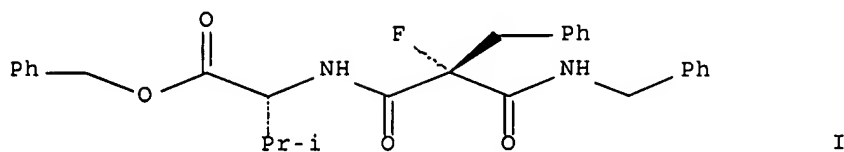
RN 160000-01-1 CAPLUS

CN D-Valine, N-[2-fluoro-1,3-dioxo-2-(phenylmethyl)-3-[(phenylmethyl)amino]propyl]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 27 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1995:30147 CAPLUS Full-text
 DOCUMENT NUMBER: 122:56436
 TITLE: Optically active fluorinated β -lactam building blocks: a novel fluorinated retroamide isostere
 AUTHOR(S): Abouabdellah, Ahmed; Welch, John T.
 CORPORATE SOURCE: Department of Chemistry, State Univ. New York, Albany, NY, 12222, USA
 SOURCE: Tetrahedron: Asymmetry (1994), 5(6), 1005-13
 CODEN: TASYE3; ISSN: 0957-4166
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



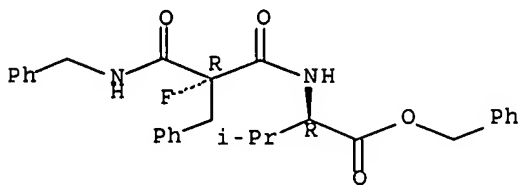
AB A new and versatile synthesis of optically active α -fluoro- malonamide derivs. from enantiomerically pure 3-fluoro-2-azetidinones is described. A fluorinated retroamide isostere, (-)-(R)- HO₂CCF(CH₂Ph)CONHCH₂Ph, was introduced into a small peptidomimetic(I) for use as an HIV-1 protease inhibitor.

IT 160000-01-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of valylfluoromalonamides)

RN 160000-01-1 CAPLUS

CN D-Valine, N-[2-fluoro-1,3-dioxo-2-(phenylmethyl)-3-[(phenylmethyl)amino]propyl]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

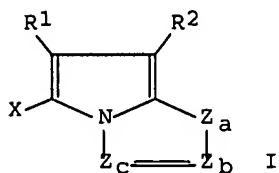
Absolute stereochemistry.



L53 ANSWER 28 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:641574 CAPLUS Full-text
 DOCUMENT NUMBER: 121:241574
 TITLE: Silver halide color photographic photosensitive material
 INVENTOR(S): Nakagawa, Hajime; Shimada, Yasuhiro
 PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 73 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05297538	A	19931112	JP 1992-121080	19920416
PRIORITY APPLN. INFO.: GI			JP 1992-121080	19920416



AB The title material contains ≥ 1 kind(s) of cyan couplers I ($Z_a = \text{NH}$, CHR3; Z_b , $Z_c = \text{CR}_4$, N; R_1 -3 = electron-withdrawing group having a Hammett's substituent constant $\sigma_p > 0.20$; the sum of the σ_p values of R_1 and R_2 is > 0.65 ; $R_4 = \text{H}$, substrate, if there are > 2 of R_4 they may be the same or different; $X = \text{H}$, group to be eliminated upon coupling; R_1 -4 or X may become a divalent group and bond with a polymer which is larger than a dimer or a polymer chain to form a homopolymer or a copolymer) and ≥ 1 kind(s) of development inhibitor-releasing couplers A- $\{(L_1)a-(B)m\}p-(L_2)n$ -DI [A = group which splits $\{(L_1)a-(B)m\}p-(L_2)n$ -DI upon reaction with an oxidized aromatic primary amine developing agent; L_1 = group which splits the bond at its right side (the bond with $(B)n$) after breaking the bond at its left side; B = group which splits the bond at its right side upon reaction with an oxidized developing agent; L_2 = group which splits the bond at its right side (the bond with DI) after breaking the bond at its left side; DI = development inhibitor; $a, m, n = 0, 1$; $p = 0-2$, when p is plural $(L_1)a-(B)m$ may be the same or different]. The material shows good color reproducibility and superior shelf life.

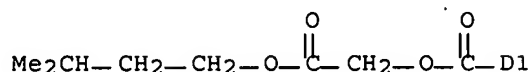
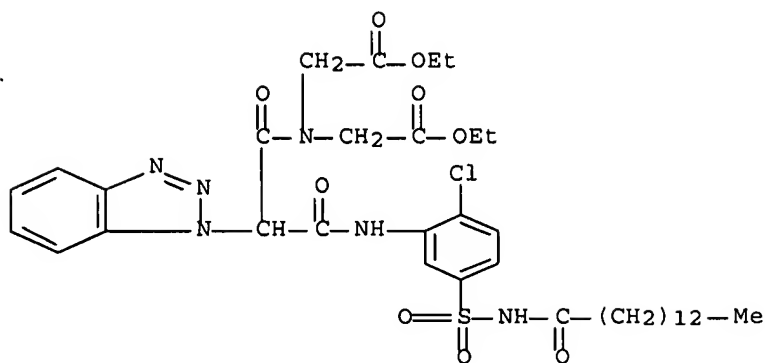
IT 158372-17-9

RL: USES (Uses)

(photog. development inhibitor-releasing coupler)

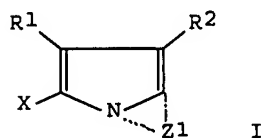
RN 158372-17-9 CAPLUS

CN 1H-Benzotriazolecarboxylic acid, 1-[1-[[bis(2-ethoxy-2-oxoethyl)amino]carbonyl]-2-[[2-chloro-5-[[[(1-oxotetradecyl)amino]sulfonyl]phenyl]amino]-2-oxoethyl]-, 2-(3-methylbutoxy)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 29 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:495837 CAPLUS Full-text
 DOCUMENT NUMBER: 121:95837
 TITLE: Silver halide color photographic materials with
 excellent color reproducibility and storage stability
 INVENTOR(S): Nakagawa, Hajime; Yamakawa, Kazuyoshi
 PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 75 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05281680	A	19931029	JP 1992-108460	19920402
PRIORITY APPLN. INFO.: GI			JP 1992-108460	19920402



AB The Ag halide color photog. material, comprising ≥ 1 red-, green-, and blue-sensitive Ag halide emulsion layers on a support, contains a cyan coupler I [R1 = H, substituent; R2 = substituent; X = H, moiety released upon coupling reaction with oxidation products of color developing agent; Z1 = nonmetallic atomic group forming N-containing 6-membered heterocyclyl; heterocyclyl contains ≥ 1 dissociating moiety] and a DIR coupler A- $\{(L1)a-(B)n\}p-(L2)n$ -DI [A

= moiety releasing {(L1)a-(B)n}p-(L2)n-DI upon reacting with aromatic primary amine developing agent; L1 = moiety released from A and then from B; B = moiety released from L2 upon reaction with oxidation products of developing agent; L2 = moiety released from C and then from DI; DI = development inhibitor; a, m, n = 0, 1; p = 0-2].

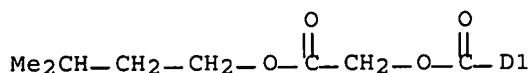
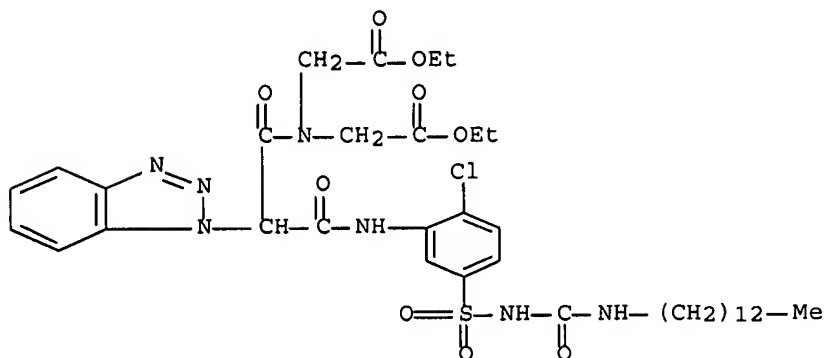
IT 156343-04-3

RL: USES (Uses)

(silver halide color photog. material containing)

RN 156343-04-3 CAPLUS

CN 1H-Benzotriazolecarboxylic acid, 1-[1-[[bis(2-ethoxy-2-oxoethyl)amino]carbonyl]-2-[[2-chloro-5-[[[(tridecylamino)carbonyl]amino]sulfonyl]phenyl]amino]-2-oxoethyl]-, 2-(3-methylbutoxy)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 30 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:482789 CAPLUS Full-text

DOCUMENT NUMBER: 121:82789

TITLE: Acid-aided reactions of 3-acylamino-β-lactams: some observations

AUTHOR(S): Sanjayan, Gangadhar J.; Mukerjee, Arya K.

CORPORATE SOURCE: Fac. Sci., Banaras Hindu Univ., Varanasi, 221 005, India

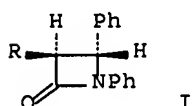
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1994), 33B(1), 76-8

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

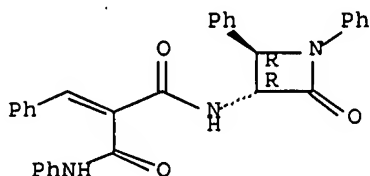
GI



IT 156486-82-7

RN 156486-82-7 CAPLUS

Relative stereochemistry.
Double bond geometry unknown.



PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 568037	A1	19931103	EP 1993-106891	19930428
EP 568037	B1	19981104		
R: BE, DE, FR, GB, NL				
JP 05307248	A	19931119	JP 1992-134523	19920428
JP 2835665	B2	19981214		
US 5459024	A	19951017	US 1995-400269	19950303
PRIORITY APPLN. INFO.:			JP 1992-134523	A 19920428
			US 1993-52670	B1 19930427
OTHER SOURCE(S):		MARPAT 121:46485		

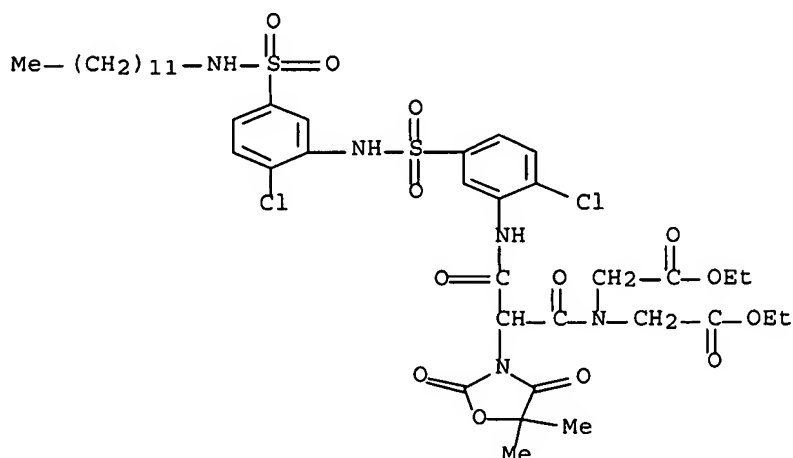
AB The present invention relates to silver halide color photog. materials having improved sharpness, higher photog. speeds and increased fastness by forming images in the presence of couplers wherein the rate of dye formation is high, the color forming d. is high and the dye which is formed has a high degree of fastness. A photog. coupler represented by the formula $R_1R_2NCOCHXCONH_2SO_2NR_3R_4$ wherein R_1 and R_2 each independently represents an alkyl group, an aryl group or a heterocyclic group, R_3 represents a hydrogen atom, an alkyl group, an aryl group or a heterocyclic group, X represents a group which can be eliminated when the coupler reacts with an oxidized product of a primary aromatic amine developing agent, Z represents a phenylene group, R_4 represents an aryl group or a heterocyclic group, and R_1 and R_2 , R_3 and Z , or R_3 and R_4 may be linked to form a ring is contained in at least one hydrophilic colloid layer of the silver halide color photog. materials.

IT 155926-64-0

RL: TEM (Technical or engineered material use); USES (Uses)
(photog. coupler)

RN 155926-64-0 CAPLUS

CN Glycine, N-[N-[2-chloro-5-[[[2-chloro-5-[(dodecylamino)sulfonyl]phenyl]amino]sulfonyl]phenyl]-2-(5,5-dimethyl-2,4-dioxo-3-oxazolidinyl)-3-oxo- β -alanyl]-N-(2-ethoxy-2-oxoethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 32 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:539079 CAPLUS Full-text

DOCUMENT NUMBER: 119:139079

TITLE: Preparation of (pyrrolidinoethyl)urea derivatives as analgesics

INVENTOR(S): Takeuchi, Makoto; Takayama, Kazuhisa; Onda, Kenichi; Motoie, Hiroyuki; Isomura, Yasuo

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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GI



IT

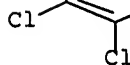
IT

RN

RN

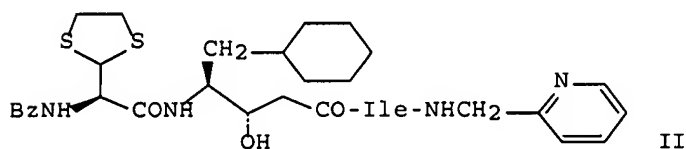
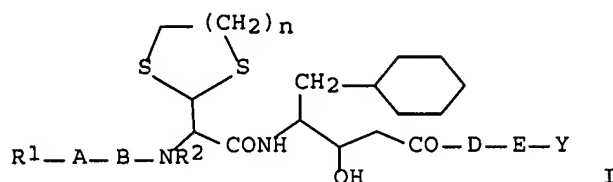
CN

Ab



ACCESSION NUMBER: 1992:612973 CAPLUS Full-text
 DOCUMENT NUMBER: 117:212973
 TITLE: Renin-inhibiting peptides of the cyclohexylstatine type
 INVENTOR(S): Bender, Wolfgang; Schmidt, Gunter; Knorr, Andreas; Stasch, Johannes Peter
 PATENT ASSIGNEE(S): Bayer A.-G., Germany
 SOURCE: Ger. Offen., 61 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

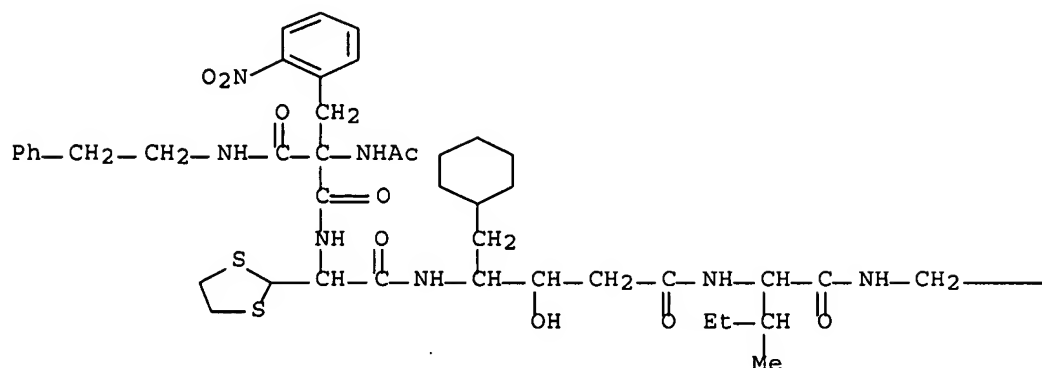
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4038921	A1	19920611	DE 1990-4038921	19901206
WO 9210509	A1	19920625	WO 1991-EP2300	19911203
W: AU, BG, BR, CA, CS, FI, HU, JP, KR, NO, PL, RO, SU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
AU 9190252	A	19920708	AU 1991-90252	19911203
JP 06503315	T	19940414	JP 1992-500344	19911203
PRIORITY APPLN. INFO.:			DE 1990-4038921	A 19901206
			WO 1991-EP2300	A 19911203
OTHER SOURCE(S):			MARPAT 117:212973	
GI				



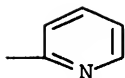
AB Peptides I [A, B, D, E = bond, (un)protected amino acid; R1 = H, protective group, acyl; R2 = H, alkyl, CH2Ph; R1-A-B-NR2 = heterocyclic; Y = H, alkyl, cycloalkyl, protective group) (un)substituted NH2; n = 1, 2] were prepared as plasma renin inhibitors (no data). Thus, peptide II was obtained from amino(dithiolene)acetic acid in 4 steps.
 IT 144165-68-4P 144299-10-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 144165-68-4 CAPLUS
 CN L-threo-Pentonamide, 4-[[N-[N-acetyl-2-nitro-α-[[2-phenylethyl]amino]carbonyl]-D-phenylalanyl]-L-2-(1,3-dithiolan-2-yl)glycyl]amino]-5-cyclohexyl-2,4,5-trideoxy-N-[2-methyl-1-[[2-

pyridinylmethyl)amino]carbonyl]butyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

PAGE 1-A

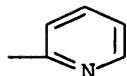
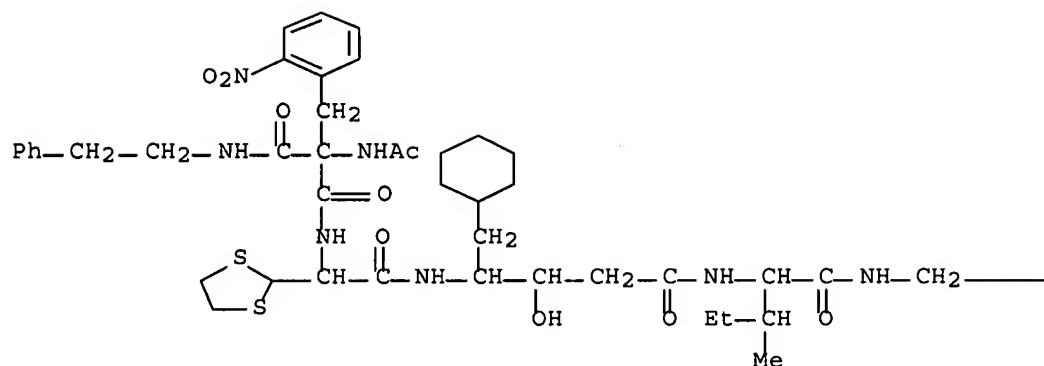


PAGE 1-B



RN 144299-10-5 CAPLUS

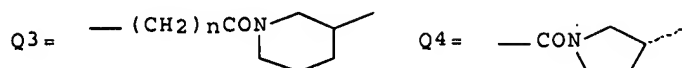
CN L-threo-Pentonamide, 4-[N-[N-acetyl-2-nitro- α -[[2-phenylethyl)amino]carbonyl]-L-phenylalanyl]-L-2-(1,3-dithiolan-2-yl)glycyl]amino]-5-cyclohexyl-2,4,5-trideoxy-N-[2-methyl-1-[[2-pyridinylmethyl)amino]carbonyl]butyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



L53 ANSWER 34 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1992:129634 CAPLUS Full-text
 DOCUMENT NUMBER: 116:129634
 TITLE: Preparation of amidino derivatives of peptides and amino acids as drugs
 INVENTOR(S): Alig, Leo; Edenhofer, Albrecht; Mueller, Marcel; Trzeciak, Arnold; Weller, Thomas
 PATENT ASSIGNEE(S): Hoffmann-La Roche, F., A.-G., Switz.
 SOURCE: Eur. Pat. Appl., 28 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 445796	A2	19910911	EP 1991-103462	19910307
EP 445796	A3	19911030		
EP 445796	B1	19980617		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 2037153	A1	19910910	CA 1991-2037153	19910226

ZA 9101534	A	19911127	ZA 1991-1534	19910301
HU 56582	A2	19910930	HU 1991-186	19910304
AU 9172086	A	19920820	AU 1991-72086	19910304
AU 646838	B2	19940310		
IL 97401	A	19950315	IL 1991-97401	19910304
US 5273982	A	19931228	US 1991-665110	19910305
FI 9101148	A	19910910	FI 1991-1148	19910307
JP 04217652	A	19920807	JP 1991-65316	19910307
JP 2501252	B2	19960529		
RU 2072359	C1	19970127	RU 1991-4894657	19910307
AT 167482	T	19980715	AT 1991-103462	19910307
ES 2118067	T3	19980916	ES 1991-103462	19910307
NO 9100934	A	19910910	NO 1991-934	19910308
NO 301167	B1	19970922		
BR 9100941	A	19911105	BR 1991-941	19910308
PRIORITY APPLN. INFO.:			CH 1990-775	A 19900309
			CH 1991-115	A 19910117
			CH 1991-192	19910123
OTHER SOURCE(S):	MARPAT 116:129634			
GI				



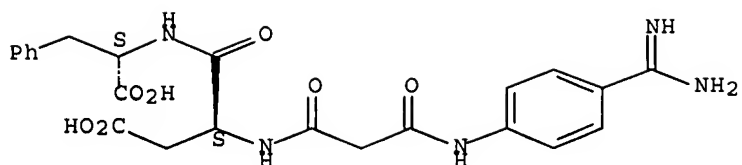
AB H2N(HN:)C-X-Y-CO-Z-CH(Q1)CO2Q2 [Q1 = H, Me, Ph; Q2 = H, phenylalkyl, physiol. cleavable alkyl; X = phenylene, pyridylene, piperidinylene; Y = CH2CH2NHCOCH2, NHCO(CH2)3, Q3, Q4, etc.; n = 0-2; Z = piperazinylene, piperidinylene, NHCH2, NHCHMe, etc.], were prepared Thus, H-β-Ala-Asp(OCMe3)-Phe-OCMe3 (preparation given) was condensed with 4-NCC6H4CO2H to give the N-cyanobenzoyl derivative, which was treated with H2S in pyridine/Et3N to give the N-thiocarbamoylbenzoyl derivative The latter was refluxed with MeI in acetone and the product was refluxed with NH4OAc in MeOH to give the protected N-amidinobenzoyl derivative, which was treated with CF3CO2H to give N-[N-[N-(p-amidinobenzoyl)-β-alanyl]-α-aspartyl]-3-phenylalanine trifluoroacetate. The latter inhibited fibrinogen binding to its receptor (glycoprotein IIb/IIIa) with IC50 = 0.003 μM.

IT 138107-62-7P 138108-00-6P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as drug)

RN 138107-62-7 CAPLUS

CN L-Phenylalanine, N-[N-[N-[4-(aminoiminomethyl)phenyl]-3-oxo-β-alanyl]-L-α-aspartyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 138108-00-6 CAPLUS

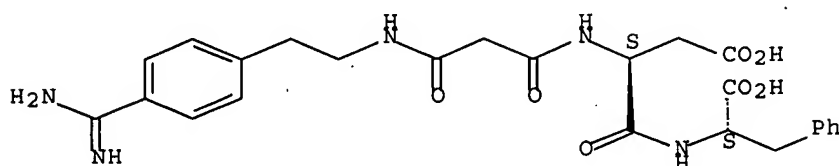
CN L-Phenylalanine, N-[N-[N-[2-[4-(aminoiminomethyl)phenyl]ethyl]-3-oxo-beta-alanyl]-L-alpha-aspartyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 138107-99-0

CMF C25 H29 N5 O7

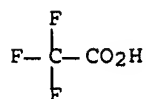
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



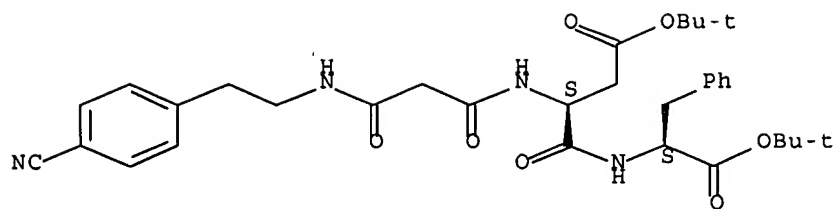
IT 138135-00-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as drug intermediate)

RN 138135-00-9 CAPLUS

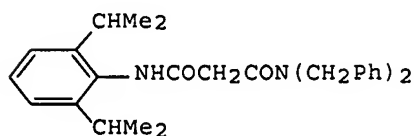
CN L-Phenylalanine, N-[N-[N-[2-(4-cyanophenyl)ethyl]-3-oxo-beta-alanyl]-L-alpha-aspartyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 35 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1991:655831 CAPLUS Full-text
 DOCUMENT NUMBER: 115:255831
 TITLE: Preparation of N,N'-disubstituted malonamides as
 cholesterol acyltransferase inhibitors
 INVENTOR(S): Roark, William H.
 PATENT ASSIGNEE(S): Warner-Lambert Co., USA
 SOURCE: Can. Pat. Appl., 50 pp.
 CODEN: CPXXEB
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2030105	A1	19910517	CA 1990-2030105	19901115
AU 9066590	A	19910613	AU 1990-66590	19901113
FI 9005645	A	19910517	FI 1990-5645	19901114
NO 9004955	A	19910521	NO 1990-4955	19901115
EP 433662	A2	19910626	EP 1990-121904	19901115
EP 433662	A3	19910703		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 57705	A2	19911230	HU 1990-7154	19901115
ZA 9009186	A	19920729	ZA 1990-9186	19901115
CN 1051733	A	19910529	CN 1990-109182	19901116
JP 03220164	A	19910927	JP 1990-308982	19901116
PRIORITY APPLN. INFO.:			US 1989-437727	A 19891116
			US 1990-594484	A 19901009
OTHER SOURCE(S):	MARPAT 115:255831			
GI				



I

AB Title compds. ArNHCO(CH₂)_mCR₃R₄(CH₂)_nCONR₁R₂ [Ar = (CH₂)_xR; (substituted) naphthyl; R = (substituted) Ph; m, n, x = 0-2; R₃, R₄ = H, (hydroxy)C₁-10 alkyl, (amino)C₁-10 alkyl; 1 of R₃, R₄ = H and the other = amino; R₁, R₂ = H, (CH₂)_tCR₇R₈(CH₂)_wR₉, C₁-20 hydrocarbyl, (amino)C₁-6 alkyl, (carboalkoxy)C₁-6

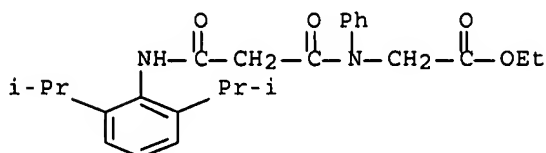
alkyl, (substituted) Ph, etc.; R7, R8 = H, C1-6 alkyl; R9 = (substituted) Ph or R8 = (substituted) Ph when R7 = H; t, w = 0-4; t + w ≤ 5] were prepared as cholesterol acyltransferase inhibitors. Thus, 2,6-diisopropylaniline was condensed with ClCOCH2CO2Et and the product was hydrolyzed to carboxymethyl amide. This was coupled with (PhCH2)2NH to give title compound I. I had IC50 of 0.013 μM against cholesterol acyltransferase. I lowered blood cholesterol by 42 mg/dL in rats.

IT 137379-32-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as cholesterol acyltransferase inhibitor)

RN 137379-32-9 CAPLUS

CN Glycine, N-[3-[[2,6-bis(1-methylethyl)phenyl]amino]-1,3-dioxopropyl]-N-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 36 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:123053 CAPLUS Full-text

DOCUMENT NUMBER: 114:123053

TITLE: Synthesis of human renin inhibitory peptides, angiotensinogen transition-state analogs containing a retro-inverso amide bond

AUTHOR(S): Harada, Hiromu; Iizuka, Kinji; Kamijo, Tetsuhide; Akahane, Kenji; Yamamoto, Ryoji; Nakano, Yasushi; Tsubaki, Atsushi; Kubota, Tetsuhiro; Shimaoka, Iwao; et al.

CORPORATE SOURCE: Cent. Res. Lab., Kissei Pharm. Co., Ltd., Matsumoto, 399, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1990), 38(11), 3042-7

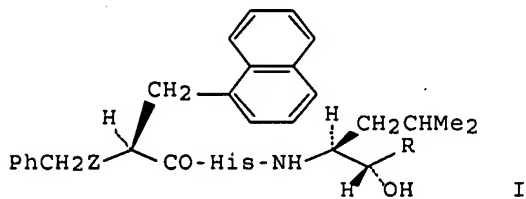
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:123053

GI

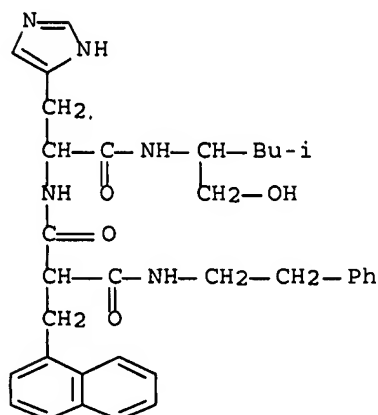


AB The exptl. details for the synthesis of human renin inhibitors I (Z = CH₂NHCOCH₂, R = H, CONHCH₂CH₂CHMe₂, CO₂Me, CH₂CO₂Me; Z = O₂CNH, CONHCH₂, CH₂NHCO, NHCOCH₂, R = H) are described. In order to avoid metabolic degradation of the Phe-His amide bond in transition-state analogs, structurally modified acyl residues were incorporated into the inhibitors. I (Z = CH₂NHCOCH₂, R = CONHCH₂CH₂CMe₂) had potent human renin inhibitory activity, and it lowered blood pressure when administered orally to common marmosets.

IT 132413-89-9P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and renin inhibitory activity of)

RN 132413-89-9 CAPLUS

CN Propanediamide, N-[2-[[1-(hydroxymethyl)-3-methylbutyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-2-(1-naphthalenylmethyl)-N'-(2-phenylethyl)-, [2S-[1[R*(R*)],2R*]]- (9CI) (CA INDEX NAME)



L53 ANSWER 37 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:526032 CAPLUS Full-text

DOCUMENT NUMBER: 113:126032

TITLE: The anti-leishmanial activity of dipeptide esters on *Leishmania amazonensis* amastigotes

AUTHOR(S): Ramazeilles, C.; Juliano, L.; Chagas, J. R.; Rabinovitch, M.

CORPORATE SOURCE: Unite Immunoparasitol., Inst. Pasteur, Paris, 75724, Fr.

SOURCE: Parasitology (1990), 100(2), 201-7
 CODEN: PARAAE; ISSN: 0031-1820

DOCUMENT TYPE: Journal

LANGUAGE: English

AB L-Amino acid esters, such as L-Leu-OMe, kill *L. amazonensis* amastigotes by a mechanism which appears to involve ester hydrolysis by cysteine proteinases located in the parasite megasomes. The killing of isolated amastigotes by L-dipeptide esters and some structure-activity correlations were demonstrated. Toxicity of the compds. for the parasites was measured by a tetrazolium (MTT) reduction assay. The results show that active dipeptide esters contained at least 1 hydrophobic amino acid (Leu, Ile, Val, Phe or Trp). The activity of

homodipeptide Me esters depended on the nature of the amino acid, as indicated by the following series: Phe-Phe-OMe > Val-Val-OMe > Leu-Leu-OMe > Trp-Trp-OMe > Ile-Ile-OMe. The nature of the amino acids in Leu-X-OMe and X-Leu-OMe was relatively unimportant when X was Phe, Trp or Val. However, when X was Ala or Gly, Leu-X-OMe was several-fold more active than X-Leu-OMe. A similar preference for the more hydrophobic residue in the amino terminal position was also found in esters containing a single phenylalanine or valine. Protection of the amino group by benzyloxycarbonyl (Z) or t-butyloxycarbonyl (BOC) substituents markedly enhanced the activity of the esters. An-mPhe-Gly-OEt, a retro-inverso analog of Bz-Phe-Gly-OEt, was several-fold more active than the parent compound. Selected esters were assayed on infected macrophages and concns. that induced minimal toxicity to the host cells were estimated. The ED50s for intracellular parasites were 1.5 to 5-fold higher than those for isolated amastigotes. Therapeutic ratios (concentration for detectable toxicity for macrophages/ED90) ranged from 1.6 (for Z-Leu-Gly-OMe) to 8 (for Val-Val-OMe).

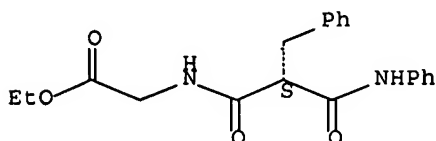
IT 129279-73-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antileishmanial activity of, on Leishmania amazonensis amastigotes, structure in relation to)

RN 129279-73-8 CAPLUS

CN Glycine, N-[1,3-dioxo-3-(phenylamino)-2-(phenylmethyl)propyl]-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 38 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:154893 CAPLUS Full-text

DOCUMENT NUMBER: 110:154893

TITLE: Preparation and testing of arylalanylhistidineamides as renin inhibitors

INVENTOR(S): Nakano, Kohji; Fujikura, Takashi; Hara, Ryuichiro; Ichihara, Masato; Fukunaga, Yikiko; Shibasaki, Masayuki

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 48 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 281316	A2	19880907	EP 1988-301609	19880225
EP 281316	A3	19900816		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FI 8800734	A	19880828	FI 1988-734	19880217
FI 89058	B	19930430		

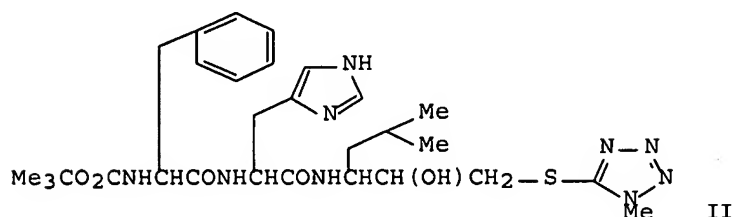
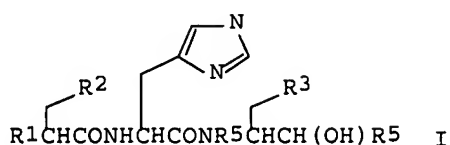
FI 89058	C	19930810		
US 4904660	A	19900227	US 1988-160173	19880225
NO 8800851	A	19880829	NO 1988-851	19880226
JP 02009865	A	19900112	JP 1988-43630	19880226
CA 1325497	C	19931221	CA 1988-560029	19880226
AU 8812502	A	19880901	AU 1988-12502	19880229
AU 612626	B2	19910718		

PRIORITY APPLN. INFO.:

	JP 1987-46454	A	19870227
	JP 1987-115144	A	19870512
	JP 1987-206146	A	19870818
	JP 1987-289017	A	19871116

OTHER SOURCE(S): CASREACT 110:154893; MARPAT 110:154893

GI

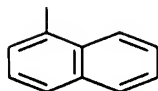
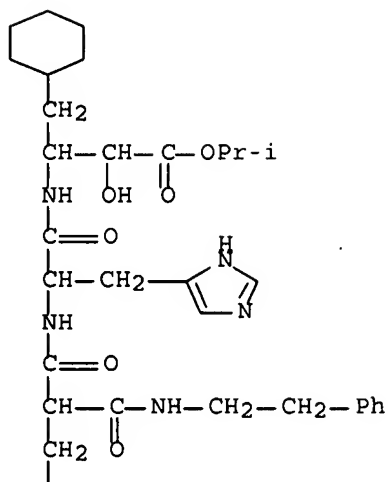


AB The title compds. [I; R1 = alkoxy-carbonyl, alkoxy-carbonylamino, (substituted) alkyl, etc.; R2 = Ph, naphthyl; R3 = C1-6 alkyl, cyclohexyl, Ph; R4 = O2NCH2, alkoxy-carbonyl, CH2S(O)nR6; R5 = H, C1-6 alkyl; R6 = (substituted) heterocyclyl; n = 0-2] useful as renin inhibitors, were prepared BOC-Phe-His-NHNH2 in DMF at -10° was treated with HCl/dioxane/isoamyl nitrite; the mixture was stirred 30 min at -30° and N-methylmorpholine was added. 3-Amino-5-methyl-1-(1-methyl-5-tetrazolylthio)-2-hexanol in DMF was added and the mixture was kept overnight in a cold room to give peptide derivative II. I inhibited human plasma renin with IC50 values of 5 + 10-10 to 4 + 10-9 M.

IT 119832-39-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of, as renin inhibitor)

RN 119832-39-2 CAPLUS

CN L-Histidinamide, 2-(1-naphthalenylmethyl)-3-oxo-N-(2-phenylethyl)-β-alanyl-N-[1-(cyclohexylmethyl)-2-hydroxy-3-(1-methylethoxy)-3-oxopropyl]-(9CI) (CA INDEX NAME)



L53 ANSWER 39 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:412218 CAPLUS Full-text

DOCUMENT NUMBER: 105:12218

TITLE: Stability-indicating assay for oxyphenbutazone. Part II. High-performance liquid chromatographic determination of oxyphenbutazone and its degradation products

AUTHOR(S): Fabre, Huguet; Ramiamana, Andrianandrasana;

CORPORATE SOURCE: Blanchin, Marie Dominique; Mandrou, Bernadette
Lab. Chim. Anal., Fac. Pharm., Montpellier, 34060, Fr.

SOURCE: Analyst (Cambridge, United Kingdom) (1986), 111(2), 133-7

CODEN: ANALAO; ISSN: 0003-2654

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An HPLC method is proposed for the simultaneous determination of oxyphenbutazone (I) [129-20-4] and 6 potential decomposition products, using a reversed-phase column and UV detection. The method is more sensitive than thin-layer chromatog. and allows the determination of 0.1% of each degradation product (with respect to I). It was applied to the anal. of com. tablets, capsules, and ointments.

IT 102712-77-6

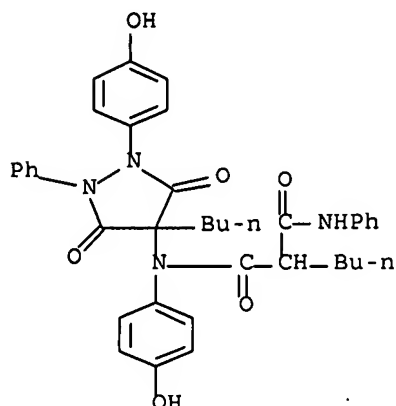
RL: ANT (Analyte); ANST (Analytical study)

(determination of, in presence of oxyphenbutazone, in pharmaceuticals by

HPLC)

RN 102712-77-6 CAPLUS

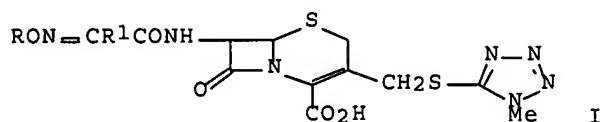
CN Propanediamide, 2-butyl-N-[4-butyl-1-(4-hydroxyphenyl)-3,5-dioxo-2-phenyl-4-pyrazolidinyl]-N-(4-hydroxyphenyl)-N'-phenyl- (9CI) (CA INDEX NAME)



L53 ANSWER 40 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1984:510633 CAPLUS Full-text
 DOCUMENT NUMBER: 101:110633
 TITLE: Cephalosporins
 INVENTOR(S): Engel Masoliver, Carlos; Inchaurredo Lasagaboster, Fermin
 PATENT ASSIGNEE(S): Laboratorios Fher S. A., Spain
 SOURCE: Span., 13 pp.
 CODEN: SPXXAD
 DOCUMENT TYPE: Patent
 LANGUAGE: Spanish
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 518223	A1	19840116	ES 1982-518223	19821215
PRIORITY APPLN. INFO.:			ES 1982-518223	19821215

GI



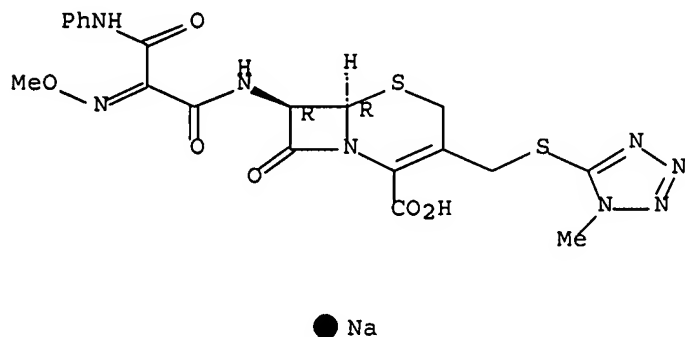
AB Cephalosporins I (R = alkyl; R1 = cyano, carbamoyl, alkoxy-carbonyl) were prepared. Thus, MeO2CCH2CONPh was converted to MeO2CC(:NOH)CONHPh which was methylated and hydrolyzed to give HO2CC(:NOMe)CONHPh (II). I (R = Me, R1 = CONPh) was obtained by acylating the aminocephem with II.
 IT 91530-42-6P 91530-43-7P 91530-47-1P
 RL: SPN (Synthetic preparation); PREP (Preparation of preparation of)

RN 91530-42-6 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[2-(methoxyimino)-1,3-dioxo-3-(phenylamino)propyl]amino]-3-[[[(1-methyl-
1H-tetrazol-5-yl)thio]methyl]-8-oxo-, monosodium salt, (6R-trans)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

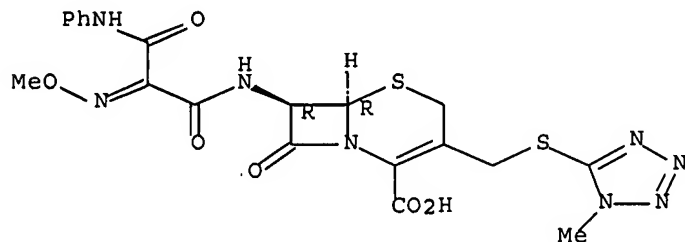


RN 91530-43-7 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[2-(methoxyimino)-1,3-dioxo-3-(phenylamino)propyl]amino]-3-[[[(1-methyl-
1H-tetrazol-5-yl)thio]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

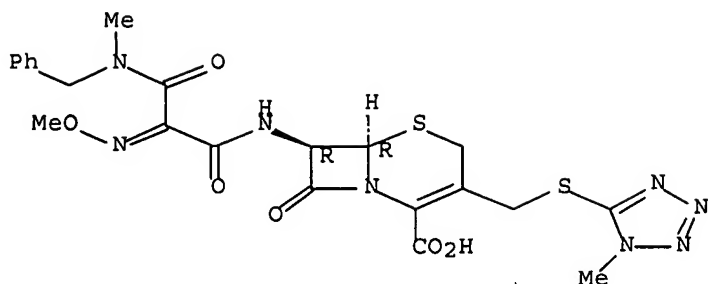


RN 91530-47-1 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[2-(methoxyimino)-3-[methyl(phenylmethyl)amino]-1,3-dioxopropyl]amino]-
3-[[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, (6R-trans)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

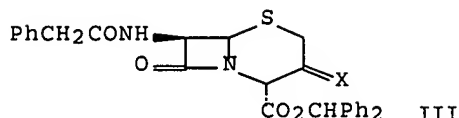
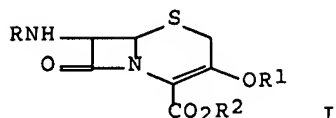


L53 ANSWER 41 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1984:34336 CAPLUS Full-text
 DOCUMENT NUMBER: 100:34336
 TITLE: Cephalosporin ethers
 INVENTOR(S): Scartazzini, Riccardo; Bickel, Hans
 PATENT ASSIGNEE(S): Ciba-Geigy Corp. , USA
 SOURCE: U.S., 41 pp. Cont.-in-part of U.S. Ser. No. 373,818,
 abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4405778	A	19830920	US 1976-657904	19760213
CH 587268	A5	19770429	CH 1972-9788	19720629
CH 603666	A5	19780831	CH 1977-1154	19720629
CH 605987	A5	19781013	CH 1972-18722	19721222
CH 605988	A5	19781013	CH 1973-2655	19730223
ZA 7304050	A	19740529	ZA 1973-4050	19730614
SU 542474	A3	19770105	SU 1973-1940203	19730627
SU 677662	A3	19790730	SU 1973-1943362	19730627
AT 7305696	A	19750815	AT 1973-5696	19730628
AT 329745	B	19760525		
ES 416411	A1	19760516	ES 1973-416411	19730628
ES 416412	A1	19760516	ES 1973-416412	19730628
ES 416413	A1	19761116	ES 1973-416413	19730628
HU 172459	B	19780928	HU 1973-CI1599	19730628
PL 93779	B1	19770630	PL 1973-163718	19730629
PL 104396	B1	19790831	PL 1973-173571	19730629
PL 116789	B1	19810630	PL 1973-163715	19730629
NO 7500055	A	19740103	NO 1975-55	19750108
ES 442262	A1	19770701	ES 1975-442262	19751031
CH 597241	A5	19780331	CH 1976-5624	19760505
FI 7902808	A	19790910	FI 1979-2808	19790910
FI 64941	B	19831031		
FI 64941	C	19840210		
PRIORITY APPLN. INFO.:			CH 1972-9788	A 19720629
			CH 1972-12195	A 19720817
			CH 1972-18722	A 19721222
			CH 1973-2655	A 19730223
			US 1973-373818	A2 19730626
			CH 1972-2655	A 19730223

CH 1973-7388	A 19730523
FI 1973-1751	A 19730530
NO 1973-2683	A 19730628
CH 1976-5624	A 19760505

OTHER SOURCE(S): MARPAT 100:34336
GI



AB Cephalosporins I (R = acyl; R1 = alkyl; R2 = ester group) were prepared Thus, I (R = PhCH2CO, R1 = Me, R2 = CHPh2) (II) was prepared by ozonolysis of III (X = CH2) and methylation of the resulting mixture of III (X = O) and its 1-oxide. III (X = CH2) was prepared from Na 7- phenylacetamidocephalosporanate by deacetylation, esterification, iodination, and deiodination. II was deacylated, hydrolyzed to the acid, and reacylated to give numerous acyl derivs.

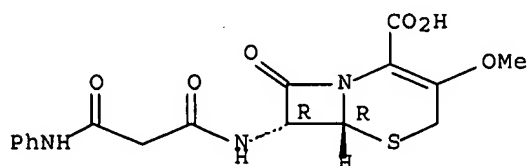
IT 51803-52-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51803-52-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methoxy-8-oxo-, (6R-trans)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 42 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:558866 CAPLUS Full-text

DOCUMENT NUMBER: 99:158866

TITLE: Amino acid derivatives and their therapeutic use

INVENTOR(S): Roques, Bernard; Schwart, Jean Charles; Lecomte, Jeanne Marie

PATENT ASSIGNEE(S): Fr.

SOURCE: Eur. Pat. Appl., 105 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 82088	A1	19830622	EP 1982-402314	19821216
EP 82088	B1	19860402		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
FR 2518088	A1	19830617	FR 1981-23488	19811216
FR 2518088	B1	19871127		
JP 58150547	A	19830907	JP 1982-221060	19821216
JP 03046463	B	19910716		
AT 18902	T	19860415	AT 1982-402314	19821216
US 4618708	A	19861021	US 1985-715764	19850325
US 4738803	A	19880419	US 1986-900814	19860822
PRIORITY APPLN. INFO.:			FR 1981-23488	A 19811216
			US 1982-449687	A1 19821214
			EP 1982-402314	A 19821216
			US 1985-715764	A3 19850325

OTHER SOURCE(S): CASREACT 99:158866; MARPAT 99:158866

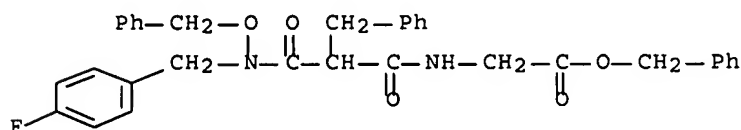
AB R-X-Y-Z-CHR1COR2 [R = phosphono, sulfo, amino, carbamoyl, alkyl; X = CH(CH2)nR3 (n = 0-2; R3 = H, (un)substituted alkyl, Ph, naphthyl, cyclohexyl, thienyl, etc.), C:CHR3; Y = CO, NH, CH2CO; Z = CO, NR4 (R4 = alkyl, R1R4 = a ring); R1 = H or (un)substituted alkyl or Ph; R2 = OH or (un)substituted alkyl, phenoxy, amino, etc.] were prepared (101 compds. claimed). Thus, reaction of PhCH2CHBrCO2H with PhCH2ONH2, followed by formylation and coupling with glycine benzyl ester tosylate gave PhCH2ON(CHO)CH(CH2Ph)CO-Gly-OCH2Ph. The products are useful as enkephalinase inhibitors, analgesics, antidepressants, antidiuretics, and hypotensives. Thus, HON(CHO)CH2CH(CH2Ph)CO-Gly-NHCH2C6H4F-p was an effective analgesic, countering the effects of phenylbenzoquinone at 1 mg/kg i.v.

IT 87438-32-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)

RN 87438-32-2 CAPLUS

CN Glycine, N-[N-[(4-fluorophenyl)methyl]-3-oxo-N-(phenylmethoxy)-2-(phenylmethyl)-β-alanyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L53 ANSWER 43 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:562688 CAPLUS Full-text

DOCUMENT NUMBER: 97:162688

TITLE: Cephalosporins

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

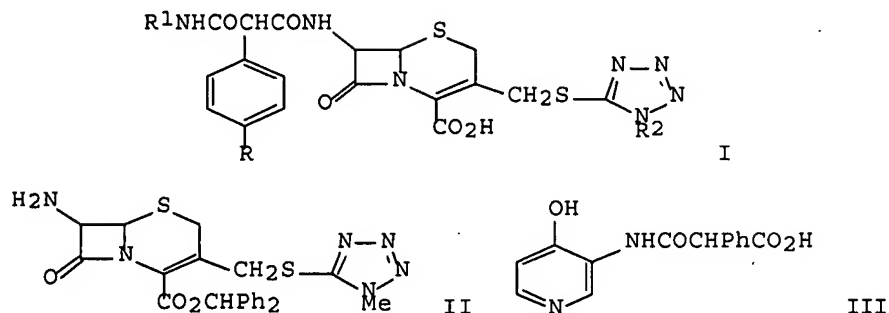
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 57080390	A	19820519	JP 1980-155394	19801105
PRIORITY APPLN. INFO.:			JP 1980-155394	19801105
OTHER SOURCE(S):	CASREACT 97:162688			
GI				



AB Antibiotics I [R = H, OH; R1 = (substituted) Ph, pyridyl, pyrimidyl, quinolinyl; R2 = alkyl] were prepared by, e.g., acylation of II. Thus, stirring 136 mg III with 250 mg II in DMF containing dicyclohexylcarbodiimide at room temperature for 1 h gave 193 mg I (R = H, R1 = 4-hydroxy-3-pyridyl, R2 = Me) benzhydryl ester, which on hydrolysis gave 136 mg I (R = H, R1 = 4-hydroxy-3-pyridyl, R2 = Me). Min. inhibition concns. are given for I against *Escherichia coli*, *Proteus mirabilis*, *Serratia marcescens* and *Staphylococcus aureus*.

IT 83255-30-5P 83255-37-2P

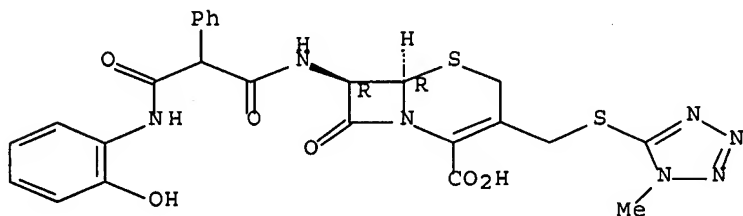
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antibacterial activity of)

RN 83255-30-5 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[3-[(2-hydroxyphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-3-[[1-methyl-1H-tetrazol-5-yl]thio]methyl]-8-oxo-, [6R-(6 α ,7 β)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

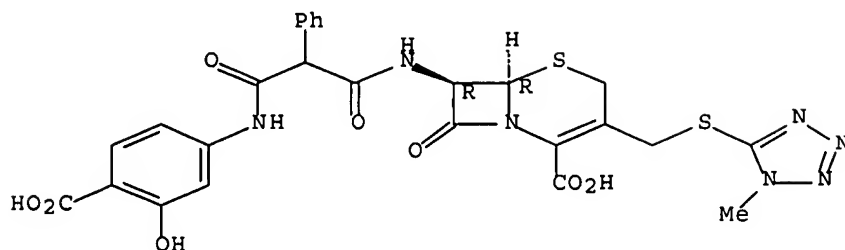


RN 83255-37-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[3-[(4-carboxy-3-hydroxyphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-3-[[1-methyl-1H-tetrazol-5-yl]thio]methyl]-8-oxo-, [6R-(6 α ,7 β)]-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 44 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:402717 CAPLUS Full-text

DOCUMENT NUMBER: 97:2717

TITLE: Potent cephalosporinase inhibitors:

7 β -[2-(1,3-dithiolan-2-ylidene)acetamido]cephalosporins and related compounds

AUTHOR(S): Ohya, Satoshi; Miyadera, Tetsuo; Yamazaki, Mitsuo

CORPORATE SOURCE: Biol. Res. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan

SOURCE: Antimicrobial Agents and Chemotherapy (1982), 21(4), 613-17

CODEN: AMACCQ; ISSN: 0066-4804

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Cephalosporins possessing a 1,3-dithiolane, 1,3-dithiane, or 1,3-dithietane ring on their 7 β -substituents showed potent inhibitory activity against cephaloridine hydrolysis by cephalosporinases purified from *Proteus morganii*, *P. rettgeri*, and *P. inconstans*, which were not inhibited by clavulanic acid, a well-known β -lactamase inhibitor. The mode of inhibition was competitive. The dithiolane cephalosporins themselves were stable against hydrolysis by the β -lactamases tested. A combination of a dithiolane cephalosporin and cephaloridine synergistically inhibited in vitro growth of strains of *P. morganii*, *P. rettgeri*, *P. inconstans*, *Enterobacter aerogenes*, *E. cloacae*, and *Serratia marcescens*.

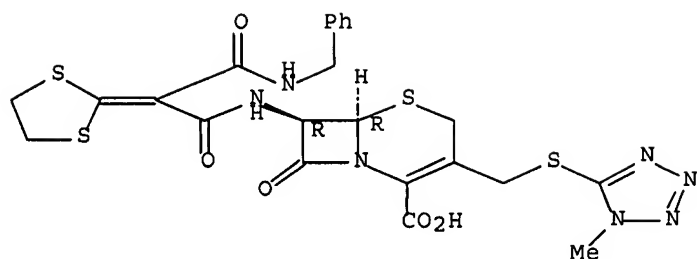
IT 81948-88-1

RL: BIOL (Biological study)
(cephalosporinase inhibition by)

RN 81948-88-1 CAPLUS

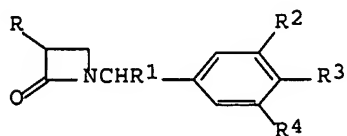
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[2-(1,3-dithiolan-2-ylidene)-1,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]-3-[[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, (6R-trans)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 45 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1981:65461 CAPLUS Full-text
 DOCUMENT NUMBER: 94:65461
 TITLE: 4-Unsubstituted azetidinone derivatives
 INVENTOR(S): Hashimoto, Masashi; Hemmi, Keiji; Kamiya, Takashi;
 Komori, Tadaaki; Nakaguti, Osamu; Saito, Yoshihisa;
 Shiokawa, Youichi; Takasugi, Hisahi; Takaya, Takao;
 Teraji, Tsutomu
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
 SOURCE: U.S., 130 pp. Cont.-in-part of U.S. Ser. No. 694,891,
 abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4207234	A	19800610	US 1977-858375	19771207
US 4472300	A	19840918	US 1980-130205	19800313
PRIORITY APPLN. INFO.:			US 1975-593668	A2 19750707
			US 1976-694891	A2 19760610
			US 1977-858375	A3 19771207
OTHER SOURCE(S):	CASREACT 94:65461; MARPAT 94:65461			
GI				

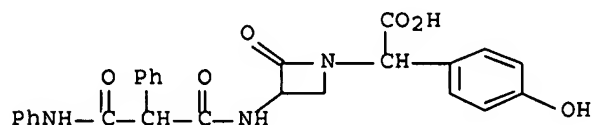


AB Lactacillanic acids and analogs I (R = NH₂, acylamino, benzenesulfonamido; R₁ = CO₂H, pharmaceutically acceptable salt or ester derivative of CO₂H; R₂ = H, NH₂, NO₂, halo, alkoxy, alkylthio; R₃ = H, OH, alkyl, alkylthio, OCH₂Ph; R₄ = H, Halo, alkoxy, alkylthio), which showed bactericidal activity, were prepared Thus, 3-aminolactacillanic acid reacted with PhCH₂COCl in water-Me₂CO containing NaHCO₃ to yield I (R = PhCH₂CONH, R₁ = CO₂H, R₃ = OH, R₂ = R₄ = H).
 IT 59510-12-2P 59510-40-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 59510-12-2 CAPLUS

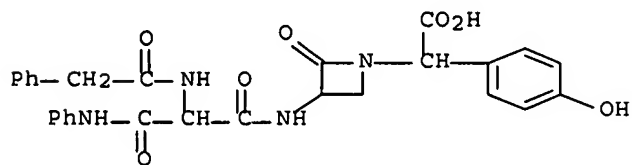
CN 1-Azetidineacetic acid, 3-[[1,3-dioxo-2-phenyl-3-(phenylamino)propyl]amino]- α -(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 59510-40-6 CAPLUS

CN 1-Azetidineacetic acid, 3-[[1,3-dioxo-2-[(phenylacetyl)amino]-3-(phenylamino)propyl]amino]- α -(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



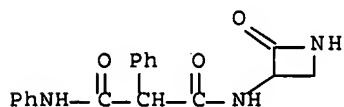
● Na

IT 75263-61-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(N-alkylation of)

RN 75263-61-5 CAPLUS

CN Propanediamide, N-(2-oxo-3-azetidiny)-N',2-diphenyl- (9CI) (CA INDEX NAME)



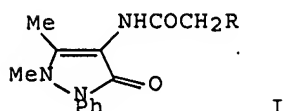
L53 ANSWER 46 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:405150 CAPLUS Full-text

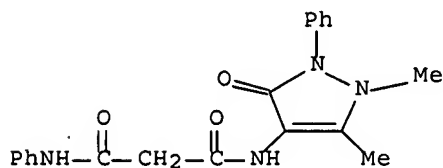
DOCUMENT NUMBER: 91:5150

TITLE: Synthesis of 4-(N-substituted-carbamoylacetylamido)phenazones, 4-(substituted-

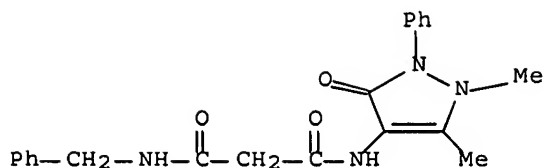
AUTHOR(S): hydrazidocarbonylacetamido)phenazones and
 N1-(4-phenazonylcarbamoylacetyl)-N2-aroylehydrazines
 Abou-Ouf, A. A.; Farghaly, A. M.; El-Kerdawy, M. M.;
 Massoud, A.
 CORPORATE SOURCE: Fac. Pharm., Univ. Mansoura, Mansoura, Egypt
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1978),
 16B(11), 989-91
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB 4-Malonamidophenazone Et ester I (R = CO₂Et) (II), prepared by the hydrolysis
 of 4-(2-cyanoacetamido)phenazone I (R = CN) followed by esterification,
 underwent condensation with R₁NH₂ (R₁ = H, Me, Et, Pr, Ph, PhCH₂ 4-EtOC₆H₄)
 gave I (R = CONHR₁). The hydrazide I (R = CONHNH₂) (III), prepared by the
 reaction of H₂NNH₂ on II, reacts with R₂COR₃ (R₂ = H, Me; R₃ = Ph, substituted
 Ph) to give I (R = CONHN:CR₂R₃). The reaction of III with R₄Cl (R₄ = Bz,
 PhSO₂, etc.) in pyridine or C₆H₆-Et₃N gives the corresponding aroylehydrazines
 I (R = CONHNHR₄). Preliminary pharmacol. screening shows promising results.
 IT 70373-56-7P 70373-57-8P 70373-58-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 70373-56-7 CAPLUS
 CN Propanediamide, N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-
 yl)-N'-phenyl- (9CI) (CA INDEX NAME)

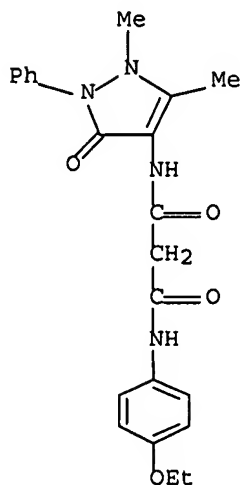


RN 70373-57-8 CAPLUS
 CN Propanediamide, N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-
 yl)-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



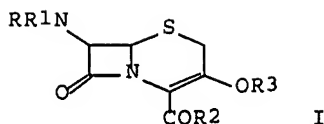
RN 70373-58-9 CAPLUS

CN Propanediamide, N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-N'-(4-ethoxyphenyl)- (9CI) (CA INDEX NAME)



L53 ANSWER 47 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1979:152207 CAPLUS Full-text
 DOCUMENT NUMBER: 90:152207
 TITLE: Enol ethers of 7-β-aminocephem-3-ol-4-carboxylic acid derivatives
 INVENTOR(S): Scartazzini, Riccardo; Bickel, Hans
 PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
 SOURCE: Patentschrift (Switz.), 31 pp. Addn. to Swiss 587,268.
 CODEN: SWXXAS
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 605989	A5	19781013	CH 1973-7387	19730523
PRIORITY APPLN. INFO.: GI			CH 1973-7387	A 19730523



AB The title ethers I [R = NH₂-protecting group; R₁ = H, acyl; RR₁ = bivalent protective group; R₂ = CO₂H-protecting group; R₃ = (substituted) hydrocarbon group] and their 1-oxides and salts were prepared by the reaction of I (R₃ = H) or the corresponding ketone with an ester of R₃OH with H₂SO₄, halosulfonic acid or haloalkanesulfonic acid. Thus, I (R = Me₃CO₂CCHPhCO, R₁ = R₃ = H, R₂ = OCHPh₂) reacted with F₃CSO₃Me in CH₂Cl₂ to give I (R-R₂ = same, R₃ = Me).

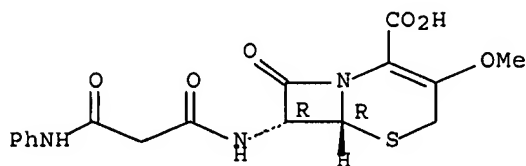
IT 51803-52-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51803-52-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methoxy-8-oxo-, (6R-trans)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 48 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:500769 CAPLUS Full-text

DOCUMENT NUMBER: 89:100769

TITLE: Synthesis for preparation of α -carboxyl and
 α -carboxy-amido penicillanic and cephalosporanic
acid derivatives

AUTHOR(S): Huhn, Magda; Dvortsak, Peter; Zalantai, Livia
CORPORATE SOURCE: Chinoim Chem. and Pharm. Works Ltd., Budapest, Hung.
SOURCE: Curr. Chemother., Proc. Int. Congr. Chemother., 10th
(1978), Meeting Date 1977, Volume 1, 569-72.
Editor(s): Siegenthaler, Walter; Luethy, Ruedi. Am.
Soc. Microbiol.: Washington, D. C.
CODEN: 37XLA2

DOCUMENT TYPE: Conference

LANGUAGE: English

AB A series of the title derivs. was prepared and tested in vitro for antimicrobial activity. Most derivs. acylated with malonic acids and with hemianilides of phenylmalonic acid showed remarkable activity against Mycobacterium tuberculosis, and gram.-pos. and -neg. microorganisms. In vivo, however, none of the test compds. significantly prolonged the survival time of mice infected i.v. with mycobacteria, even after administration of s.c. doses of 200 mg/kg over 10 days.

IT 60657-76-3 67371-57-7 67371-58-8

67371-59-9 67371-60-2

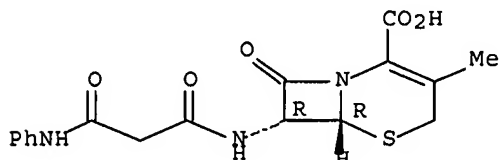
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(tuberculostatic activity of)

RN 60657-76-3 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-, (6R-trans)-
(9CI) (CA INDEX NAME)

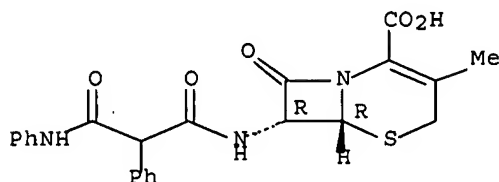
Absolute stereochemistry.



RN 67371-57-7 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-2-phenyl-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-,
[6R-(6 α ,7 β)]- (9CI) (CA INDEX NAME)

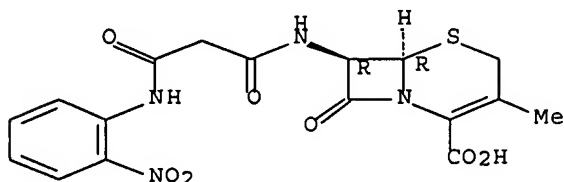
Absolute stereochemistry.



RN 67371-58-8 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-methyl-7-[[3-[(2-nitrophenyl)amino]-1,3-dioxopropyl]amino]-8-oxo-,
(6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

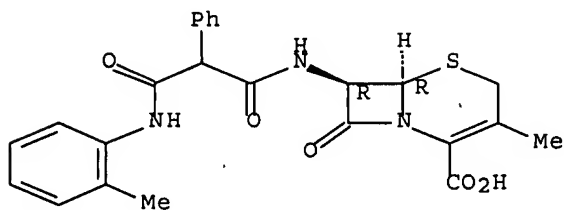


RN 67371-59-9 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-methyl-7-[[3-[(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-8-oxo-, [6R-(6 α ,7 β)]- (9CI) (CA INDEX NAME)

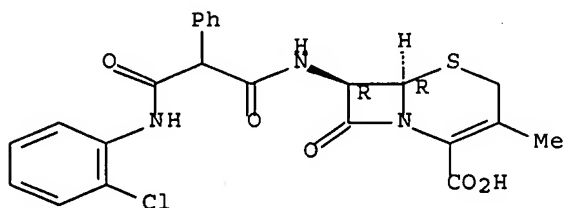
Absolute stereochemistry.



RN 67371-60-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[3-[(2-chlorophenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-3-methyl-8-oxo-, [6R-(6 α ,7 β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 49 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:27732 CAPLUS Full-text

DOCUMENT NUMBER: 88:27732

TITLE: 4-Hydroxyphenylbutazone: a potentially immunogenic
contaminant of phenylbutazone preparations

AUTHOR(S): Bundgaard, Hans

CORPORATE SOURCE: Dep. Pharm., R. Dan. Sch. Pharm., Copenhagen, Den.

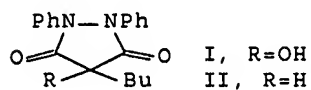
SOURCE: Archiv for Pharmaci og Chemi, Scientific Edition
(1977), 5(4), 87-96

CODEN: AVPCCS; ISSN: 0302-248X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



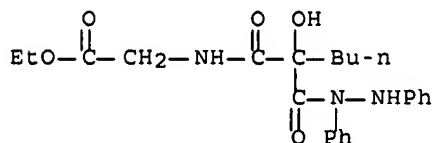
butyltartronic acid mono-N,N'-diphenylhydrazide amides
[RNHCOC(Bu)(OH)CONHNHPh]. An irreversible reaction with serum albumin took place at alkaline pH. The contaminant reacted .apprx.25-fold more readily with glycylglycine [556-50-3] than benzylpenicillin and was potentially an immunogenic substance, possibly involved in clin. allergic reactions to I prepsns.

IT 64725-03-7

RL: BIOL (Biological study)
(as hydroxyphenylbutazone aminolysis product, in phenylbutazone pharmaceuticals)

RN 64725-03-7 CAPLUS

CN Hexanoic acid, 2-[[[(2-ethoxy-2-oxoethyl)amino]carbonyl]-2-hydroxy-, 1,2-diphenylhydrazide (9CI) (CA INDEX NAME)



L53 ANSWER 51 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:535287 CAPLUS Full-text

DOCUMENT NUMBER: 87:135287

TITLE: Acylation of 6-aminopenicillanic acid, 7-aminocephalosporanic acid, and 7-aminodeacetoxycephalosporanic acid and their derivatives

INVENTOR(S): Diago Meseguer, Jose; Fernandez Lizarbe, Jose Ramon; Palomo Coll, Antonio Luis; Zugaza Bilbao, Alvaro

PATENT ASSIGNEE(S): Gema S. A., Spain; Antibioticos S. A.

SOURCE: Ger. Offen., 31 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

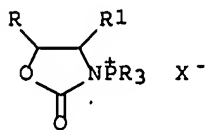
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2701751	A1	19770721	DE 1977-2701751	19770118
ES 444470	A1	19770516	ES 1976-444470	19760120
NL 7700570	A	19770722	NL 1977-570	19770120
PRIORITY APPLN. INFO.:			ES 1976-444470	A 19760120

GI



I

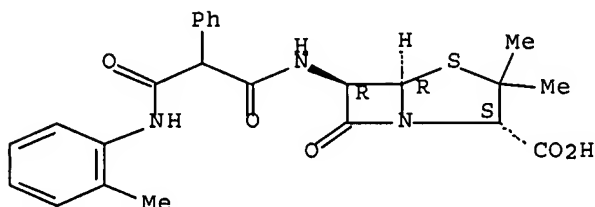
AB The title acids were acylated with 2,5-(O₂N)₂C₆H₄CO₂H, thienylacetic acid, PhCHClCO₂H, N₃CHPhCO₂H, etc; by preparing a salt of the acylating acid with an organic base, e.g., Et₃N, which was treated with I (R = Cl, Br, Me₂N, R = R₁ = H, Me; X = Br, Cl) to give a mixture of active species with varying content of acid chloride, N-acyl-2-oxazolidinone, and 2-acyloxy-Δ²-oxazoline. The title acids were then added to this mixture to give the N-acyl derivative

IT 34093-30-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 34093-30-6 CAPLUS

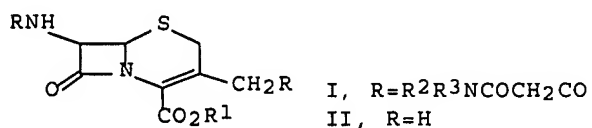
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[3-[(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-7-oxo-, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 52 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1976:543125 CAPLUS Full-text
 DOCUMENT NUMBER: 85:143125
 TITLE: Cephalosporins
 INVENTOR(S): Shibuya, Chisei; Ito, Hirataka; Usubuchi, Yutaka; Yamawaki, Naokuni; Ichikawa, Yasushi
 PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51054578	A	19760513	JP 1974-127562	19741107
PRIORITY APPLN. INFO.: GI			JP 1974-127562	A 19741107



AB Cephalosporins I (R = H, OH, alkanoyloxy, quaternary ammonium, thiadiazolylthio, tetrazolylthio, etc.; R1 = H, alkyl, aralkyl, trisubstituted silyl, phenacyl, alkanoyloxymethyl, salt-forming ion, etc., or RR11 form a lactam ring; R2 and R3 = H, alkyl, aryl, aralkyl, heterocyclyl, alkoxy carbonyl, etc., or R2R3 = alkylene, alkenylene, but not R2 = H and R3 = aliphatic hydrocarbon group) were prepared by acylating II with acids R2R3NCOCH2CO2H or their reactive derivs. I are antibacterial agents (no data). Thus, 0.93 g PhNHCOCH2CO2H was treated with ClCO2Et and then with 1.33 g II (R = H, R1 = CMe3) and Et3N in CHCl3 to give 2.12 g I (R = R2 = H, R1 = CMe3, R3 = Ph). Deprotection with CF3CO2H gave I (R = R1 = R2 = H, R3 = Ph). Also prepared was I (R = OAc, R1 = H, R2 = Me, R3 = Ph).

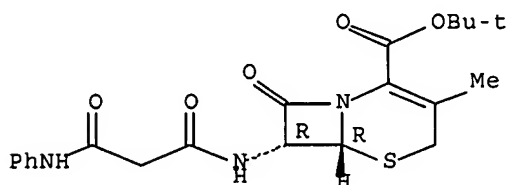
IT 60657-75-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)

RN 60657-75-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-,
1,1-dimethylethyl ester, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



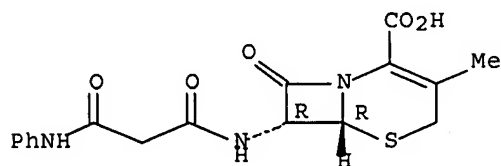
IT 60657-76-3P 60657-77-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 60657-76-3 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methyl-8-oxo-, (6R-trans)-
(9CI) (CA INDEX NAME)

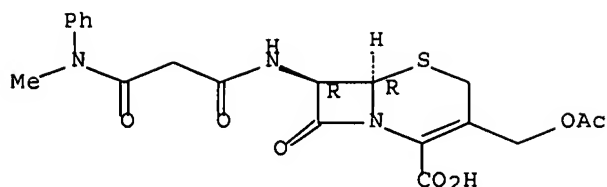
Absolute stereochemistry.



RN 60657-77-4 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid;
3-[(acetyloxy)methyl]-7-[[3-(methylphenylamino)-1,3-dioxopropyl]amino]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



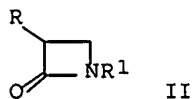
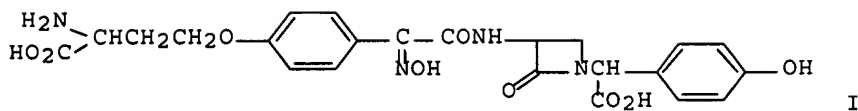
L53 ANSWER 53 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1976:421078 CAPLUS Full-text
 DOCUMENT NUMBER: 85:21078
 TITLE: Azetidinone derivatives
 INVENTOR(S): Kamiya, Takashi; Yoshihisa, Takarazuka; Hashimoto, Masashi; Teraji, Tsutomu; Takaya, Takao; Komori, Tadaaki; Nakaguti, Osamu; Oku, Teruo; Shiokawa, Youichi; et al.
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
 SOURCE: Ger. Offen., 318 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2529941	A1	19760408	DE 1975-2529941	19750704
JP 51125061	A	19761101	JP 1974-77091	19740704
JP 51125062	A	19761101	JP 1974-85526	19740724
JP 51125064	A	19761101	JP 1974-88452	19740731
JP 51075056	A	19760629	JP 1975-2650	19741223
BE 830934	A1	19760102	BE 1975-157924	19750702
CH 618161	A5	19800715	CH 1975-8634	19750702
DK 7503023	A	19760105	DK 1975-3023	19750703
FI 7501949	A	19760105	FI 1975-1949	19750703
NO 7502419	A	19760106	NO 1975-2419	19750703
FR 2278335	A1	19760213	FR 1975-20990	19750703
FR 2278335	B1	19821217		
SE 428799	B	19830725	SE 1975-7683	19750703
SE 428799	C	19831103		
NL 7508008	A	19760106	NL 1975-8008	19750704
AU 7582778	A	19770106	AU 1975-82778	19750704
ES 439134	A1	19770301	ES 1975-439134	19750704
ZA 7504306	A	19770525	ZA 1975-4306	19750704
GB 1519495	A	19780726	GB 1975-28394	19750704
HU 172476	B	19780928	HU 1975-FU336	19750704
AT 7505170	A	19790715	AT 1975-5170	19750704
AT 355034	B	19800211		
CA 1063108	A1	19790925	CA 1975-230828	19750704
AT 7806099	A	19790915	AT 1978-6099	19780822
AT 7806098	A	19800415	AT 1978-6098	19780822
AT 359514	B	19801110		
SE 7903460	A	19790419	SE 1979-3460	19790419
SE 7903504	A	19790420	SE 1979-3504	19790420
CH 637924	A5	19830831	CH 1980-5357	19800711

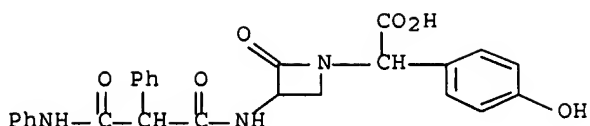
PRIORITY APPLN. INFO.:

JP	1974-77091	A	19740704
JP	1974-85526	A	19740724
JP	1974-88452	A	19740731
JP	1975-2650	A	19741223
JP	1974-100159	A	19740830
JP	1974-101712	A	19740902
JP	1974-102288	A	19740904
JP	1974-136561	A	19741126
JP	1974-138137	A	19741129
JP	1975-3779	A	19741225
JP	1975-1272	A	19741228
JP	1975-16584	A	19750207
JP	1975-18241	A	19750212
JP	1974-30356	A	19750312
JP	1975-30356	A	19750312
JP	1975-32702	A	19750317
JP	1975-32703	A	19750317
JP	1975-33292	A	19750318
JP	1975-34830	A	19750319
JP	1975-33821	A	19750320
JP	1975-33822	A	19750320
CH	1975-8634	A	19750702
AT	1975-5170	A	19750704

GI



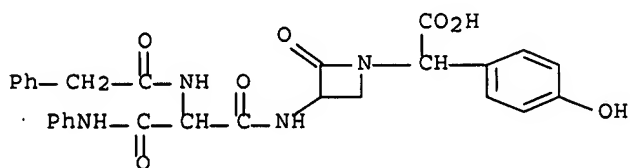
AB	After the antibiotic FR-1923 (obtained from fermentation liquor of <i>Nocardia</i>) was identified as I, 543 analogs [II; R = NH ₂ or acylamino; R ₁ = alkyl (saturated or unsatd., straight-chain or branched) with substituents, e.g., CO ₂ H (or its derivs.), CN, OH, NH ₂ , Ph or substituted Ph] were prepared by standard procedures and shown to be effective against, e.g., <i>Bacillus subtilis</i> , <i>Escherichia coli</i> , and <i>Staphylococcus aureus</i> .
IT	59510-12-2P 59510-40-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
RN	59510-12-2 CAPLUS
CN	1-Azetidineacetic acid, 3-[[1,3-dioxo-2-phenyl-3-(phenylamino)propyl]amino]- α -(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 59510-40-6 CAPLUS

CN 1-Azetidineacetic acid, 3-[[1,3-dioxo-2-[(phenylacetyl)amino]-3-(phenylamino)propyl]amino]-α-(4-hydroxyphenyl)-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)



● Na

L53 ANSWER 54 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1975:514441 CAPLUS Full-text

DOCUMENT NUMBER: 83:114441

TITLE: 7-(N-Acylamino)-2,2-dimethyl-3-cephem-4-carboxylic acids and their esters

INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter, Heinrich; Scartazzini, Riccardo

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Patentschrift (Switz.), 25 pp.

CODEN: SWXXAS

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

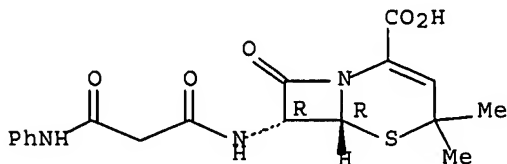
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 562250	A5	19750530	CH 1970-8472	19700605
ES 391895	A1	19730701	ES 1971-391895	19710603
NL 7107730	A	19711207	NL 1971-7730	19710604
PRIORITY APPLN. INFO.:			CH 1970-8472	A 19700605

GI For diagram(s), see printed CA Issue.

AB Cephems I (R = H₂NCHPh, MeO₂CCH₂, EtO₂CCH₂, BrCH₂, PhNHCOCH₂, MeOCH₂, 4-aminopyridiniummethyl, PhOCH₂, 4-MeC₆H₄SCH₂, AcCH₂, BzCH₂, NCCH₂, NCCHMe, NCCHPh, ClCH₂CH₂NH, ClCH₂CH₂, ClCH₂, Cl₂CH, allyl, PhCH₂, 2-thienylmethyl, MeSCH₂, (MeO₂C)₂CH, HO₂CCHPh, amino(2-thienyl)methyl, 1-tetrazolylmethyl, 1-methyl-2-imidazolylmethyl, 1,2,4-triazol-3-ylthiomethyl, BF₂CH, N₃CH₂) were prepared by acylating the 7-aminocephem, prepared from penicillins G or V in 15 steps.

IT 35621-40-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 35621-40-0 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-,
 (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

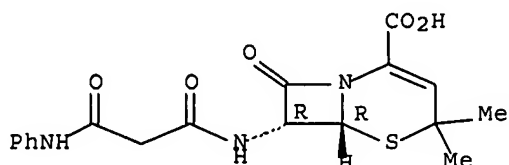


L53 ANSWER 55 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1974:437556 CAPLUS Full-text
 DOCUMENT NUMBER: 81:37556
 TITLE: 7-Amino-2,2-dimethylceph-3-em-4-carboxylic acid
 derivatives
 INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter,
 Heinrich; Scartazzini, Riccardo
 PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
 SOURCE: Brit., 50 pp.
 CODEN: BRXXAA
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1353326	A	19740515	GB 1971-5052	19710219
PRIORITY APPLN. INFO.:			GB 1971-5052	A 19710219

GI For diagram(s), see printed CA Issue.
 AB Thirty-four title compds. I (R = H, acyl; R1 = H, Me, CMe3, CH2COC6H4Br-p, Na), useful as bactericides were prepared Me2SO oxidation of the azetidinones II (R = PhCH2-CO, PhOCH2CO; R1 = CMe3), prepared from penicillin G and V, resp., gave the corresponding title compds. I which on hydrolysis and deacylation gave I (R = R1 = H). Most I (R = acyl) were prepared by acylation of I (R = R1 = H).
 IT 35621-40-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 35621-40-0 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-,
 (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 56 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1974:108513 CAPLUS Full-text
 DOCUMENT NUMBER: 80:108513
 TITLE: Isoxazolyll derivatives of penicillin and cephalosporin
 PATENT ASSIGNEE(S): Koninklijke Nederlandsche Gist- en Spiritusfabriek N.
 V.
 SOURCE: Ger. Offen., 73 pp. Division of Ger. Offen. 2,155,081
 (CA 77;48483b).
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2166468	A1	19740214	DE 1971-2166468	19711105
US 3891635	A	19750624	US 1971-195482	19711103
BE 775012	A1	19720505	BE 1971-110230	19711105
NL 7115231	A	19720509	NL 1971-15231	19711105
FR 2112504	A5	19720616	FR 1971-39822	19711105
FR 2112504	B1	19751031		
ZA 7107433	A	19720726	ZA 1971-7433	19711105
HU 162822	B	19730428	HU 1971-KO2471	19711105
AU 7135431	A	19730510	AU 1971-35431	19711105
ES 396720	A1	19750416	ES 1971-396720	19711105
CA 983920	A1	19760217	CA 1971-126985	19711105
CH 572935	A5	19760227	CH 1975-14002	19711105
CH 572936	A5	19760227	CH 1975-14003	19711105
CH 573436	A5	19760315	CH 1971-16162	19711105
SU 520050	A3	19760630	SU 1971-1713952	19711105
JP 52012200	B	19770405	JP 1971-88177	19711105
CA 993442	A2	19760720	CA 1973-166365	19730319
ES 423795	A1	19761216	ES 1974-423795	19740301
US 4010264	A	19770301	US 1974-533708	19741217
PRIORITY APPLN. INFO.:			GB 1970-53040	A 19701106
			US 1971-195482	A2 19711103
			CA 1971-126985	A3 19711105

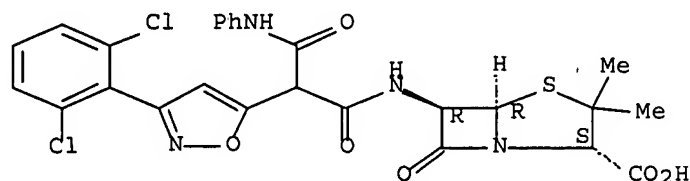
GI For diagram(s), see printed CA Issue.
 AB Penicillins I (R = 2,6-Cl₂C₆H₃, 2,4,6-Me₃C₆H₂, 4-O₂NC₆H₄, 1-adamantanyl, Me; R₁ = H, Me, CO₂H, CONH₂, CN; R₂ = H, Cl, Me, NHCO₂CH₂C₆H₄NO₂-p, NH₂, CONH₂, CONHPh) and their salts were prepared by converting 6-aminopenicillanic acid to its trimethylsilyl ester followed by treatment with the isoxazolyllacetyl chloride or by treating trimethylsilyl 6-isocyanatopenicillanate with the isoxazolyllacetic acid. The cephalosporins II (R = 2,6-Cl₂C₆H₃, 2,4,6-Me₃C₆H₂, 4-O₂NC₆H₄, Me; R₁ = H, Me; R₃ = H, OAc) were similarly prepared
 IT 36923-10-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 36923-10-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[2-[3-(2,6-dichlorophenyl)-5-isoxazolyl]-1,3-dioxo-3-(phenylamino)propyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-(2 α ,5 α ,6 β)]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



● Na

L53 ANSWER 57 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:108511 CAPLUS Full-text
DOCUMENT NUMBER: 80:108511
TITLE: Penicillin and cephalosporin derivatives
PATENT ASSIGNEE(S): Koninklijke Nederlandsche Gist- en Spiritusfabriek N. V.
SOURCE: Ger. Offen., 75 pp. Division of Ger. Offen. 2,155,081 (CA 77;48483b).
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

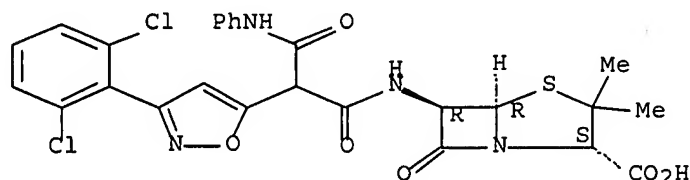
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2166467	A1	19740214	DE 1971-2166467	19711105
US 3891635	A	19750624	US 1971-195482	19711103
BE 775012	A1	19720505	BE 1971-110230	19711105
NL 7115231	A	19720509	NL 1971-15231	19711105
FR 2112504	A5	19720616	FR 1971-39822	19711105
FR 2112504	B1	19751031		
ZA 7107433	A	19720726	ZA 1971-7433	19711105
HU 162822	B	19730428	HU 1971-KO2471	19711105
AU 7135431	A	19730510	AU 1971-35431	19711105
ES 396720	A1	19750416	ES 1971-396720	19711105
CA 983920	A1	19760217	CA 1971-126985	19711105
CH 572935	A5	19760227	CH 1975-14002	19711105
CH 572936	A5	19760227	CH 1975-14003	19711105
CH 573436	A5	19760315	CH 1971-16162	19711105
SU 520050	A3	19760630	SU 1971-1713952	19711105
JP 52012200	B	19770405	JP 1971-88177	19711105
CA 993442	A2	19760720	CA 1973-166365	19730319
ES 423795	A1	19761216	ES 1974-423795	19740301
US 4010264	A	19770301	US 1974-533708	19741217
PRIORITY APPLN. INFO.:			GB 1970-53040	A 19701106

US 1971-195482
CA 1971-126985

A2 19711103
A3 19711105

GI For diagram(s), see printed CA Issue.
AB Penicillins I (R = 2,6-Cl₂C₆H₃, 2,4,6-Me₃C₆H₂, 4-O₂NC₆H₄, 1-adamantanyl, Me; R₁ = H, Me, CO₂H, CONH₂, CN; R₂ = H, Cl, Me, NHCO₂CH₂C₆H₄NO₂-p, NH₂, CONH₂, CONHPh) and their salts were prepared by converting 6-amino-penicillanic acid to its trimethylsilyl ester followed by treatment with the isoxazolylacetyl chloride or by treating trimethylsilyl 6-isocyanatopenicillanate with the isoxazolylacetic acid. The cephalosporins II (R = 2,6-Cl₂C₆H₃, 2,4,6-Me₃C₆H₂, 4-O₂NC₆H₄, Me; R₁ = H, Me; R₃ = H, OAc) were similarly prepared
IT 36923-10-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36923-10-1 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[2-[3-(2,6-dichlorophenyl)-5-isoxazolyl]-1,3-dioxo-3-(phenylamino)propyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-(2 α ,5 α ,6 β)]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



● Na

L53 ANSWER 58 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:83019 CAPLUS Full-text
DOCUMENT NUMBER: 80:83019
TITLE: Enol derivatives
INVENTOR(S): Scartazzini, Riccardo; Bickel, Hans
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Ger. Offen., 263 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2331133	A1	19740117	DE 1973-2331133	19730619
DE 2331133	C2	19840412		
CH 587268	A5	19770429	CH 1972-9788	19720629
CH 603666	A5	19780831	CH 1977-1154	19720629
CH 605987	A5	19781013	CH 1972-18722	19721222
CH 605988	A5	19781013	CH 1973-2655	19730223
FI 59601	B	19810529	FI 1973-1750	19730530
FI 59601	C	19810910		
FI 59602	B	19810529	FI 1973-1751	19730530

FI 59602	C	19810910		
FI 60870	B	19811231	FI 1973-1752	19730530
FI 60870	C	19820413		
SE 417099	B	19810223	SE 1973-8234	19730612
SE 417099	C	19810611		
SE 417429	B	19810316	SE 1973-8233	19730612
SE 417429	C	19810702		
SE 417430	B	19810316	SE 1973-8235	19730612
SE 417430	C	19810702		
ZA 7304050	A	19740529	ZA 1973-4050	19730614
RO 63761	A1	19781215	RO 1973-860064	19730614
RO 64419	A2	19790310	RO 1973-86374	19730614
RO 64226	A1	19790515	RO 1973-75138	19730614
RO 73345	A1	19820909	RO 1973-84759	19730614
FR 2190418	A1	19740201	FR 1973-23235	19730626
AU 7357386	A	19750109	AU 1973-57386	19730627
GB 1435111	A	19760512	GB 1973-30537	19730627
SU 542474	A3	19770105	SU 1973-1940203	19730627
SU 677662	A3	19790730	SU 1973-1943362	19730627
BE 801597	A1	19731228	BE 1973-132845	19730628
DD 106184	A5	19740612	DD 1973-171903	19730628
DD 106187	A5	19740612	DD 1973-171906	19730628
DD 107470	A5	19740812	DD 1973-171905	19730628
AT 7305694	A	19750415	AT 1973-5694	19730628
AT 356809	B	19800527		
AT 7305695	A	19750615	AT 1973-5695	19730628
AT 356810	B	19800527		
AT 7305696	A	19750815	AT 1973-5696	19730628
AT 329745	B	19760525		
AT 7500576	A	19750815	AT 1975-576	19730628
AT 329762	B	19760525		
HU 167726	B	19751225	HU 1973-CI1393	19730628
HU 168017	B	19760228	HU 1973-CI1392	19730628
ES 416411	A1	19760516	ES 1973-416411	19730628
ES 416412	A1	19760516	ES 1973-416412	19730628
HU 169032	B	19760928	HU 1973-CI1391	19730628
ES 416413	A1	19761116	ES 1973-416413	19730628
HU 172459	B	19780928	HU 1973-CI1599	19730628
CA 1110230	A1	19811006	CA 1973-175100	19730628
NO 145240	B	19811102	NO 1973-2681	19730628
NO 145240	C	19820210		
NO 145241	B	19811102	NO 1973-2682	19730628
NO 145241	C	19820210		
NO 145242	B	19811102	NO 1973-2683	19730628
NO 145242	C	19820210		
DK 153324	B	19880704	DK 1973-3588	19730628
NL 7309136	A	19740102	NL 1973-9136	19730629
NL 7309137	A	19740102	NL 1973-9137	19730629
NL 7309139	A	19740102	NL 1973-9139	19730629
JP 49049986	A	19740515	JP 1973-74353	19730629
JP 59034716	B	19840824		
JP 49049987	A	19740515	JP 1973-74354	19730629
JP 59033598	B	19840816		
JP 49049988	A	19740515	JP 1973-74355	19730629
JP 59033599	B	19840816		
PL 91608	B1	19770331	PL 1973-163719	19730629
PL 93779	B1	19770630	PL 1973-163718	19730629
PL 104396	B1	19790831	PL 1973-173571	19730629
PL 116789	B1	19810630	PL 1973-163715	19730629
NO 7500055	A	19740103	NO 1975-55	19750108

ES 442262	A1	19770701	ES 1975-442262	19751031
CH 597241	A5	19780331	CH 1976-5624	19760505
SE 7612053	A	19761029	SE 1976-12053	19761029
SE 435289	B	19840917		
SE 435289	C	19841220		
FI 7902808	A	19790910	FI 1979-2808	19790910
FI 64941	B	19831031		
FI 64941	C	19840210		
JP 55105690	A	19800813	JP 1979-169493	19791227
JP 59034196	B	19840821		
JP 55105691	A	19800813	JP 1979-169494	19791227
JP 59051957	B	19841217		
JP 55105692	A	19800813	JP 1979-169495	19791227
JP 59038955	B	19840920		
JP 56039093	A	19810414	JP 1980-94119	19800711
JP 60019916	B	19850518		
JP 56049390	A	19810502	JP 1980-99283	19800718
JP 61008071	B	19860311		
JP 56068684	A	19810609	JP 1980-99282	19800718
JP 61008070	B	19860311		
JP 56127392	A	19811006	JP 1981-17382	19810207
JP 59007716	B	19840220		
JP 59076089	A	19840428	JP 1983-146770	19830812
JP 60054320	B	19851129		
JP 59076090	A	19840428	JP 1983-146771	19830812
JP 60053037	B	19851122		

PRIORITY APPLN. INFO.:

CH 1972-9788	A	19720629
CH 1972-12195	A	19720817
CH 1972-18722	A	19721222
CH 1973-2655	A	19730223
CH 1972-2655	A	19730223
CH 1973-7388	A	19730523
FI 1973-1751	A	19730530
NO 1973-2683	A	19730628
CH 1976-5624	A	19760505

GI For diagram(s), see printed CA Issue.

AB 7-Acylamino-3-alkoxycephemcarboxylic acids I (R = acyl, R1 = OMe, OEt, OBu, OCH2Ph, OAc) were prepared. Thus, the Na salt of I (R = PhCH2CO, R1 = CH2OH) was converted to its diphenylmethyl ester, iodinated, and dehydroiodinated to the cepham II (X = CH2), which on ozonolysis gave a mixture of II (X = O) and its 1-oxide. Treatment of the mixture with CH2N2 gave I (R = PhCH2CO, R1 = OMe), its 1-oxide, and its 2-cephem analog, which was separated by chromatog.

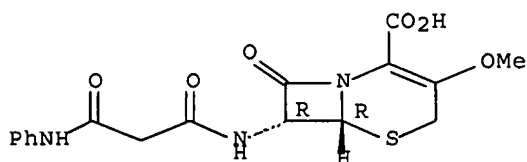
IT 51803-52-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51803-52-2 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-3-methoxy-8-oxo-, (6R-trans)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 59 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1974:82957 CAPLUS Full-text
DOCUMENT NUMBER: 80:82957
TITLE: Semisynthetic penicillins
INVENTOR(S): Palomo Coll, Antonio L.
PATENT ASSIGNEE(S): gema S. A.
SOURCE: Span., 9 pp. Addn. to Span. 376,271 (See Ger.
2,105,166 (CA 75;151782f).
CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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ES 386962	A2	19730401	ES 1970-386962	19701231
BE 762311	A1	19710701	BE 1971-99209	19710129
CH 549049	A	19740515	CH 1971-1624	19710202
DE 2105166	A	19710902	DE 1971-2105166	19710204
NL 7101575	A	19710809	NL 1971-1575	19710205
AT 314730	B	19740425	AT 1971-972	19710205
PRIORITY APPLN. INFO.:			ES 1970-376271	A 19700205
			ES 1970-386962	A 19701231

GI For diagram(s), see printed CA Issue.

AB The penicillin I (R = 0-MeC₆H₄NHCO) was prepared by treating 6-aminopenicillanic acid (II) with 0-MeC₆H₄NHCOCHPhCO₂H in the presence of Me₂N⁺:-CHCl₃.ClSO₂H. I (R = NHCONHN:CMe₂) was prepared by treating II with Me₂C:NNHCONHCHPhCO₂H. I (R = NHCONHN:CHPh) was similarly prepared

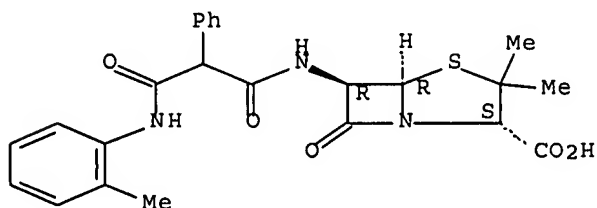
IT 34093-30-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 34093-30-6 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[3-[(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-7-oxo-, [2S-(2 α ,5 α ,6 β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 60 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1972:514397 CAPLUS Full-text
DOCUMENT NUMBER: 77:114397
TITLE: 8-Oxo-5-thia-1-azabicyclo[4,2,0]oct-2-ene compounds

INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter, Heinrich; Scartazzini, Riccardo
 PATENT ASSIGNEE(S): Ciba-Geigy A. G.
 SOURCE: S. African, 130 pp.
 CODEN: SFXXAB
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	ZA 7102523		19711125	ZA 1971-2523	19710420

GI For diagram(s), see printed CA Issue.

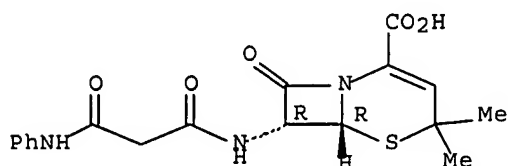
AB Tert-Bu α -[4 β -[2-(hydroxymethyl)-2-propylthio]-2-oxo-3 β -(N-phenylacetamido)-1-azetidinyll]- α -(triphenylphosphoranylidene)-acetate (I) was treated with Ac₂O in Me₂SO to give the ceph(3)-em-4-carboxylic acid (II, R = PhCH₂CO, R₁ = tert-Bu). Penicillin G azide was heated to give 2,2-dimethyl-6-(N-phenylacetamido)-3-[(2,2,2-trichloroethoxycarbonyl)amino]penam (III). III was treated with HOAc and the product treated with NaBH₄ to give 4 β -[2-(hydroxymethyl)-2-propylthio]-3 β -(N-phenylacetamido)azetidinon-2-one, which was converted to I. About 40 II (R = PhOCH₂CO, H, PhCHNH₂CO, MeO₂CCH₂CO, BrCH₂CO, PhNHCOCH₂CO, NCCH₂CO, H₂C:CHCH₂CO, 2-thienylacetyl, MeSCH₂CO, 2-imidazolylthioacetyl etc.; R₁ = tert-Bu, H, p-BrC₆H₄COCH₂) were prepared

IT 35621-40-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 35621-40-0 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-,
 (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 61 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1972:448483 CAPLUS Full-text
 DOCUMENT NUMBER: 77:48483
 TITLE: (Isoxazolylacetamido)penicillanic and -cephalosporanic acid derivatives
 PATENT ASSIGNEE(S): Koninklijke Nederlandsche Gist- en Spiritusfabriek N. V.
 SOURCE: Ger. Offen., 79 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2155081	A	19720510	DE 1971-2155081	19711105
DE 2155081	B2	19750515		
DE 2155081	C3	19751218		
US 3891635	A	19750624	US 1971-195482	19711103
BE 775012	A1	19720505	BE 1971-110230	19711105
NL 7115231	A	19720509	NL 1971-15231	19711105
FR 2112504	A5	19720616	FR 1971-39822	19711105
FR 2112504	B1	19751031		
ZA 7107433	A	19720726	ZA 1971-7433	19711105
HU 162822	B	19730428	HU 1971-KO2471	19711105
AU 7135431	A	19730510	AU 1971-35431	19711105
ES 396720	A1	19750416	ES 1971-396720	19711105
CA 983920	A1	19760217	CA 1971-126985	19711105
CH 572935	A5	19760227	CH 1975-14002	19711105
CH 572936	A5	19760227	CH 1975-14003	19711105
CH 573436	A5	19760315	CH 1971-16162	19711105
SU 520050	A3	19760630	SU 1971-1713952	19711105
JP 52012200	B	19770405	JP 1971-88177	19711105
CA 993442	A2	19760720	CA 1973-166365	19730319
ES 423795	A1	19761216	ES 1974-423795	19740301
US 4010264	A	19770301	US 1974-533708	19741217
PRIORITY APPLN. INFO.:			GB 1970-53040	A 19701106
			US 1971-195482	A2 19711103
			CA 1971-126985	A3 19711105

GI For diagram(s), see printed CA Issue.

AB Twenty-three title compds. (I; Q = Q1 or Q2; R = 2,6-Cl₂C₆H₃, 2,4,6-Me₃C₆H₂, 1-adamantyl, p-O₂NC₆H₄, or Me; R₁ = H, CO₂H, Me, CONH₂, or CN; R₂ = H, Cl, Me, p-O₂NC₆H₄CH₂O₂CNH, NH₂, H₂NCO, or PhNHCO; R₃ = H or OAc) or their Na or cyclohexylamine salts, useful as antibiotics, were prepared by amidation of the acetyl chlorides II (X = Cl). Thus, Et₃N and Me₃SiCl were added to Q₁NH₂ in AcOEt under N at .apprx.0°, the mixture was kept 35 min, II (R = 2,6-Cl₂C₆H₃, R₁ = R₂ = H) in AcOEt added at <5°, and the mixture kept 90 min at room temperature to give 32% I (Q = Q₁ = R = 2,6-Cl₂C₆H₃, R₁ = R₂ = H) as Na salt (III). III was also obtained by reaction of II (X = OH) with Q₁NCO (Me₃Si ester) in the presence of N-vinylimidazole catalyst.

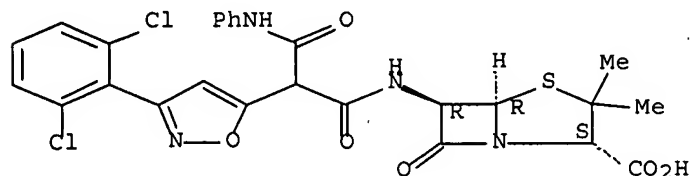
IT 36923-10-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36923-10-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[2-[3-(2,6-dichlorophenyl)-5-isoxazolyl]-1,3-dioxo-3-(phenylamino)propyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-(2 α ,5 α ,6 β)]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



● Na

L53 ANSWER 62 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1972:99686 CAPLUS Full-text

DOCUMENT NUMBER: 76:99686

TITLE: Pharmacologically active 8-oxo-5-thia-1-azabicyclo[4,2,0]oct-2-ene

INVENTOR(S): Heusler, Karl; Bickel, Hans; Fechtig, Bruno; Peter, Heinrich; Scartazzini, Riccardo

PATENT ASSIGNEE(S): Ciba-Geigy A.-G.

SOURCE: Ger. Offen., 175 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2127287	A	19711216	DE 1971-2127287	19710602
CH 563396	A5	19750630	CH 1970-8470	19700605
US 3883517	A	19750513	US 1971-149341	19710602
ES 391893	A1	19740616	ES 1971-391893	19710603
NL 7107726	A	19711207	NL 1971-7726	19710604
BE 768173	A1	19711207	BE 1971-104318	19710607
FR 2097836	A5	19720303	FR 1971-20461	19710607
FR 2100727	A1	19720324	FR 1971-20459	19710607
FR 2100727	A5	19720324		

PRIORITY APPLN. INFO.: CH 1970-8470 A 19700605
CH 1971-242 A 19710108
CH 1971-7279 A 19710517

GI For diagram(s), see printed CA Issue.

AB The cephalosporin derivs. I (R = PhCH₂, PhOCH₂, Me₃CO₂CNHCHPh, AcCH₂, EtO₂CCH₂, BrCH₂, PhNHCOCH₂, MeOCH₂, PhOCH₂, p-Me-C₆H₄SCH₂, BzCH₂, NCCH₂, NCCHMe, NCCHPr, ClCH₂CH₂NH, ClCH₂CH₂, ClCH₂, Cl₂CH, allyl, 2-thienylmethyl, MeSCH₂, (MeO₂C)₂CH, HO₂CCHPh, amino(2-thienyl)methyl, 1-tetrazolylmethyl, BrCH₂, Br₂CH, N₃CH₂, (1-methyl-2-imidazolyl)thiomethyl, 1,2,4-triazol-3-ylthiomethyl) and some esters and internal salts were prepared by cyclizing the azetidinones II (R₁ = PhCH₂CO, PhOCH₂CO), hydrolyzing to II (R₁ = H), and treating this with RCO₂H, RCO₂Na, or RCOCl. I did not undergo isomerization of the double bond owing to the 2 Me groups in the 2-position. They are active against penicillin-resistant Staphylococcus aureus.

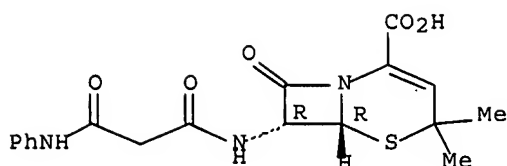
IT 35621-40-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35621-40-0 ~CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[1,3-dioxo-3-(phenylamino)propyl]amino]-4,4-dimethyl-8-oxo-,
(6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 63 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1971:551782 CAPLUS Full-text
 DOCUMENT NUMBER: 75:151782
 TITLE: α -(Carbamoyl)benzylpenicillins
 INVENTOR(S): Palomo Coll., Antonio L.
 PATENT ASSIGNEE(S): Gema S.A.
 SOURCE: Ger. Offen., 24 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2105166	A	19710902	DE 1971-2105166	19710204
ES 376271	A1	19720316	ES 1970-376271	19700205
ES 386962	A2	19730401	ES 1970-386962	19701231
PRIORITY APPLN. INFO.:			ES 1970-376271	A 19700205
			ES 1970-386962	A 19701231

GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R=Et, o-MeC₆H₄, m-F₃CC₆H₄; R₁=H or Et; NRR₁=morpholino] were prepared by reaction of 6-aminopenicillanic acid (II) with RNR₁COCHPhCO₂H and ClSO₂CH₂NH₂ Cl⁻ (III). Thus, III was added to HO₂CCHPhCONHC₆H₄Me-o in CH₂Cl₂ at -5°, stirred 1 hr at 10°, added to II in CH₂Cl₂-Et₃N-pivalic acid, and stirred with aqueous HCHO solution to give 90% I (R=o-MeC₆H₄, R₁=H). Similarly prepared were 3 other I.

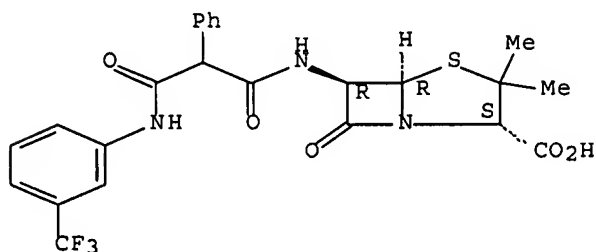
IT 34093-28-2P 34093-30-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 34093-28-2 CAPLUS

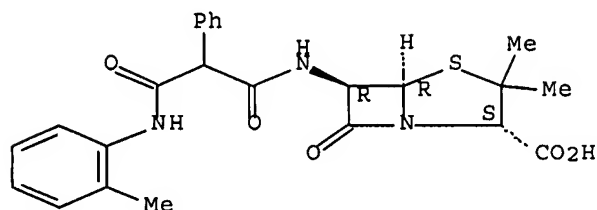
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-7-oxo-6-[2-phenyl-2-[(α,α,α -trifluoro-m-tolyl)carbamoyl]acetamido]- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 34093-30-6 CAPLUS
 CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[3-
 [(2-methylphenyl)amino]-1,3-dioxo-2-phenylpropyl]amino]-7-oxo-,
 [2S-(2 α ,5 α ,6 β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L53 ANSWER 64 OF 64 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1961:59552 CAPLUS
 DOCUMENT NUMBER: 55:59552
 ORIGINAL REFERENCE NO.: 55:11438b-e
 TITLE: Derivatives of dichloromalononic acid
 INVENTOR(S): Heymons, Albrecht; Liebig, Horst
 PATENT ASSIGNEE(S): Riedel de Haen Akt.-Ges.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

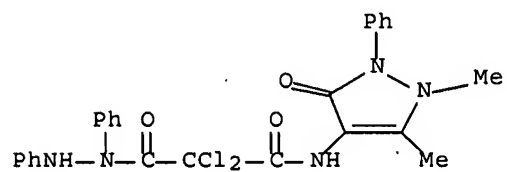
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1075628		19600218	DE	

AB Mono- and dihydrazides and cyclic monohydrazides of dichloromalononic acid, with antidiabetic action on peroral administration, were prepared by dichlorination of 3,5-dioxypyrazolidines and cleaving the product to the desired derivative by adding alcs., amines, or alkanolamines. 1,2-Diphenyl-3,5-dioxypyrazolidine (I) heated in CHCl₃ 5 hrs. at 70° with Cl passed in gave 70% 1,2-diphenyl-4,4-dichloro-3,5-dioxypyrazolidine (II), m. 112-15°. I (0.1 mole) with 0.11 mole AlCl₃ in 150 cc. CHCl₃ then Cl gave 75% II. II (1.6 g.) with 1.7 g. NaOAc and 4 cc. MeOH gave 97% dichloromalononic acid Me ester 1,2-diphenylhydrazide, m. 159°. II (3 g.) with 1 cc. pyridine and 30 cc. iso-PrOH gave 60% dichloromalononic acid iso-Pr ester 1,2-diphenylhydrazide, m. 153-66° (decomposition). II with Et₂NCH₂CH₂OH in dioxane gave 94% dichloromalononic acid diethylaminoethyl ester 1,2-diphenylhydrazide (III), m. 84-5° (decomposition). III with 0.1N HCl gave 78% dichloromalononic acid 1,2-diphenylhydrazide, m. 144-5°. II with PhNH₂ in dioxane gave 72% dichloromalononic acid anilide 1,2-diphenylhydrazide, m. 186-7°. II with 4-amino-1-phenyl-2,3-dimethyl-5-pyrazolone in dioxane gave dichloromalononic acid 1,2-diphenylhydrazide 1-phenyl-2,3-dimethyl-5-pyrazolon-4-ylamide, m. 187-93° (decomposition).

IT 114398-45-7P, Malonamic acid, N-antipyrinyl-2,2-dichloro-, 1,2-diphenylhydrazide
 RL: PREP (Preparation)
 (preparation of)

RN 114398-45-7 CAPLUS
 CN Malonamic acid, N-antipyrinyl-2,2-dichloro-, 1,2-diphenylhydrazide (6CI)

(CA INDEX NAME)



=> d his full

(FILE 'HOME' ENTERED AT 12:28:36 ON 02 MAY 2007)

FILE 'REGISTRY' ENTERED AT 12:28:58 ON 02 MAY 2007

L1 STRUCTURE UPLOADED
L2 8 SEA SSS SAM L1
D STAT QUE L2
L3 527 SEA SSS FUL L1
SAVE TEMP L3 WAR784STR1L/A

FILE 'CAPLUS' ENTERED AT 12:33:26 ON 02 MAY 2007

L4 124 SEA ABB=ON PLU=ON L3
E US2004-767784/APPS
L5 1 SEA ABB=ON PLU=ON US2004-767784/AP
D SCA
L6 1 SEA ABB=ON PLU=ON L4 AND L5
D SCA

FILE 'REGISTRY' ENTERED AT 12:35:29 ON 02 MAY 2007

L7 4 SEA ABB=ON PLU=ON L3 AND C3/ESS

FILE 'STNGUIDE' ENTERED AT 12:42:24 ON 02 MAY 2007

FILE 'REGISTRY' ENTERED AT 12:56:53 ON 02 MAY 2007
D SCA L7

FILE 'CAPLUS' ENTERED AT 12:58:13 ON 02 MAY 2007

L8 3 SEA ABB=ON PLU=ON L7

FILE 'REGISTRY' ENTERED AT 12:58:34 ON 02 MAY 2007

FILE 'STNGUIDE' ENTERED AT 12:59:14 ON 02 MAY 2007

FILE 'REGISTRY' ENTERED AT 13:02:24 ON 02 MAY 2007

L9 STRUCTURE UPLOADED
L10 4 SEA SSS SAM L9
L11 14 SEA SUB=L3 SSS SAM L9
D STAT QUE L11
L12 370 SEA SUB=L3 SSS FUL L9
SAVE TEMP L12 WAR784STR9L/A

FILE 'CAPLUS' ENTERED AT 13:07:44 ON 02 MAY 2007

L13 71 SEA ABB=ON PLU=ON L12

FILE 'REGISTRY' ENTERED AT 13:07:57 ON 02 MAY 2007

FILE 'CAPLUS' ENTERED AT 13:14:59 ON 02 MAY 2007

L14 1 SEA ABB=ON PLU=ON L12 AND L5
D SCA
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 13:15:41 ON 02 MAY 2007

L15 173 SEA ABB=ON PLU=ON (741672-55-9/BI OR 741672-56-0/BI OR
741672-57-1/BI OR 741672-58-2/BI OR 741672-59-3/BI OR 741672-60
-6/BI OR 741672-61-7/BI OR 741672-62-8/BI OR 741672-63-9/BI OR
741672-64-0/BI OR 741672-65-1/BI OR 741672-66-2/BI OR 741672-68
-4/BI OR 741672-69-5/BI OR 741672-70-8/BI OR 741672-71-9/BI OR

741672-72-0/BI OR 741672-73-1/BI OR 741672-74-2/BI OR 741672-75-3/BI OR 741672-76-4/BI OR 741672-77-5/BI OR 741672-78-6/BI OR 741672-79-7/BI OR 741672-80-0/BI OR 741672-81-1/BI OR 741672-82-2/BI OR 741672-83-3/BI OR 741672-84-4/BI OR 741672-85-5/BI OR 741672-86-6/BI OR 741672-87-7/BI OR 741672-88-8/BI OR 741672-89-9/BI OR 741672-90-2/BI OR 741672-91-3/BI OR 741672-92-4/BI OR 741672-93-5/BI OR 741672-94-6/BI OR 741672-95-7/BI OR 741672-96-8/BI OR 741672-97-9/BI OR 741672-98-0/BI OR 741672-99-1/BI OR 741673-00-7/BI OR 741673-01-8/BI OR 741673-02-9/BI OR 741673-03-0/BI OR 741673-04-1/BI OR 741673-05-2/BI OR 741673-06-3/BI OR 741673-07-4/BI OR 741673-08-5/BI OR 741673-09-6/BI OR 741673-10-9/BI OR 741673-11-0/BI OR 741673-12-1/BI OR 741673-13-2/BI OR 741673-14-3/BI OR 741673-15-4/BI OR 741673-16-5/BI OR 741673-17-6/BI OR 741673-18-7/BI OR 741673-19-8/BI OR 741673-20-1/BI OR 741673-21-2/BI OR 741673-22-3/BI OR 741673-23-4/BI OR 741673-24-5/BI OR 741673-25-6/BI OR 741673-26-7/BI OR 741673-27-8/BI OR 741673-28-9/BI OR 741673-29-0/BI OR 741673-30-3/BI OR 741673-31-4/BI OR 741673-32-5/BI OR 741673-33-6/BI OR 741673-34-7/BI OR 741673-35-8/BI OR 741673-36-9/BI OR 741673-37-0/BI OR 741673-38-1/BI OR 741673-39-2/BI OR 741673-40-5/BI OR 741673-41-6/BI OR 741673-42-7/BI OR 741673-43-8/BI OR 741673-44-9/BI OR 741673-45-0/BI OR 741673-46-1/BI OR 741673-47-2/BI OR 741673-48-3/BI OR 741673-49-4/BI OR 741673-50-7/BI OR 741673-51-8/BI OR 741673-52-9/BI OR 741673-53-0/BI OR 741673-54-1/BI OR 741

L16 FILE 'CAPLUS' ENTERED AT 13:16:13 ON 02 MAY 2007
1 SEA ABB=ON PLU=ON L15

FILE 'STNGUIDE' ENTERED AT 13:17:13 ON 02 MAY 2007

L17 FILE 'REGISTRY' ENTERED AT 13:22:27 ON 02 MAY 2007
149780 SEA ABB=ON PLU=ON NC2NC3/ESS
L18 27 SEA ABB=ON PLU=ON L17 AND L15
D SCA
E "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-O
L19 27 SEA ABB=ON PLU=ON L12 AND L17

L20 FILE 'CAPLUS' ENTERED AT 13:36:08 ON 02 MAY 2007
1 SEA ABB=ON PLU=ON L19

L21 FILE 'REGISTRY' ENTERED AT 13:38:20 ON 02 MAY 2007
197 SEA ABB=ON PLU=ON L12 NOT L15

L22 FILE 'CAPLUS' ENTERED AT 13:38:39 ON 02 MAY 2007
70 SEA ABB=ON PLU=ON L21
L23 ANALYZE PLU=ON L13 1- RN : 5445 TERMS
D

L24 FILE 'REGISTRY' ENTERED AT 13:40:57 ON 02 MAY 2007
1 SEA ABB=ON PLU=ON 146420-49-7
D SCA
L25 369 SEA ABB=ON PLU=ON L12 NOT L24

L26 FILE 'CAPLUS' ENTERED AT 13:41:49 ON 02 MAY 2007
65 SEA ABB=ON PLU=ON L25

L27 FILE 'REGISTRY' ENTERED AT 13:42:08 ON 02 MAY 2007
1 SEA ABB=ON PLU=ON 13734-34-4
D SCA
L28 1 SEA ABB=ON PLU=ON 143301-52-4

D SCA
 L29 1 SEA ABB=ON PLU=ON 147140-68-9
 D SCA
 L30 369 SEA ABB=ON PLU=ON L25 NOT (L28 OR L29)

 FILE 'CAPLUS' ENTERED AT 13:44:33 ON 02 MAY 2007
 L31 65 SEA ABB=ON PLU=ON L30

 FILE 'STNGUIDE' ENTERED AT 13:45:14 ON 02 MAY 2007

 FILE 'REGISTRY' ENTERED AT 13:48:54 ON 02 MAY 2007
 D SCA L19
 L32 0 SEA ABB=ON PLU=ON " PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-OXO-1H-1,5-BENZODIAZEPIN-3-YL)-N'-[(3,5-DIFLUOROPHENYL)METHYL]-2-METHYL-"/CN
 E "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-O
 E "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-O
 L33 1 SEA ABB=ON PLU=ON "PROPANEDIAMIDE, N-(5-BENZOYL-2,3,4,5-TETRAHYDRO-1-METHYL-2-OXO-1H-1,5-BENZODIAZEPIN-3-YL)-N'-[(3,5-DIFLUOROPHENYL)METHYL]-2-METHYL-"/CN
 D SCA

 FILE 'REGISTRY' ENTERED AT 13:51:39 ON 02 MAY 2007
 D IDE L33
 L34 STRUCTURE UPLOADED

 FILE 'MARPAT' ENTERED AT 13:55:33 ON 02 MAY 2007
 L35 9 SEA SSS SAM L9
 L36 0 SEA SSS SAM L34
 L37 2 SEA SSS FUL L34
 L38 1 SEA ABB=ON PLU=ON L37/COM

 FILE 'MARPAT' ENTERED AT 13:57:06 ON 02 MAY 2007
 D STAT QUE L38
 D IBIB ABS QHIT L38 1

 FILE 'CAPLUS' ENTERED AT 13:58:13 ON 02 MAY 2007
 L39 32 SEA ABB=ON PLU=ON GALLEY G?/AU
 L40 4 SEA ABB=ON PLU=ON GOERGLER A?/AU
 L41 297 SEA ABB=ON PLU=ON JACOBSEN H?/AU
 L42 45 SEA ABB=ON PLU=ON KITAS E?/AU
 L43 2834 SEA ABB=ON PLU=ON PETERS J?/AU
 L44 9 SEA ABB=ON PLU=ON L39 AND (L40 OR L41 OR L42 OR L43)
 L45 1 SEA ABB=ON PLU=ON L40 AND (L41 OR L42 OR L43)
 L46 1 SEA ABB=ON PLU=ON L41 AND (L42 OR L43)
 L47 3 SEA ABB=ON PLU=ON L42 AND L43
 L48 9 SEA ABB=ON PLU=ON (L44 OR L45 OR L46 OR L47)
 L49 2 SEA ABB=ON PLU=ON (L39 OR L40 OR L41 OR L42 OR L43) AND (L8 OR L26)

 FILE 'REGISTRY' ENTERED AT 14:00:33 ON 02 MAY 2007

 FILE 'CAPLUS' ENTERED AT 14:00:36 ON 02 MAY 2007
 D STAT QUE L16
 D STAT QUE L48
 D STAT QUE L49
 L50 9 SEA ABB=ON PLU=ON (L16 OR (L48 OR L49))
 D IBIB ABS HITIND L50 1-9

 FILE 'BEILSTEIN' ENTERED AT 14:01:53 ON 02 MAY 2007

L51 0 SEA SSS SAM L34
L52 0 SEA SSS FUL L34

FILE 'REGISTRY' ENTERED AT 14:02:35 ON 02 MAY 2007

FILE 'CAPLUS' ENTERED AT 14:02:38 ON 02 MAY 2007

D STAT QUE L8

D STAT QUE L26

L53 64 SEA ABB=ON PLU=ON (L8 OR L26) NOT L50
 D IBIB ABS HITSTR L53 1-64

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

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FILE CAPLUS

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FILE COVERS 1907 - 2 May 2007 VOL 146 ISS 19

FILE LAST UPDATED: 1 May 2007 (20070501/ED)

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FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 27, 2007 (20070427/UP).

FILE MARPAT

FILE CONTENT: 1961-PRESENT VOL 146 ISS 18 (20070427/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2007060644	15	MAR	2007
DE	102006023116	15	MAR	2007
EP	1762248	14	MAR	2007
JP	2007059877	08	MAR	2007
WO	2007030662	15	MAR	2007
GB	2429975	14	MAR	2007
FR	2890657	16	MAR	2007
RU	2295953	27	MAR	2007
CA	2556850	24	FEB	2007

Expanded G-group definition display now available.

FILE BEILSTEIN

FILE LAST UPDATED ON April 02, 2007

FILE COVERS 1771 TO 2006.

FILE CONTAINS 9,882,697 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.	*
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE	*
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE	*
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.	*
* FOR PRICE INFORMATION SEE HELP COST	*

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* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

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